

Figure S1. Distribution of values for the geometric characteristics of the structures under study during the MD experiment:

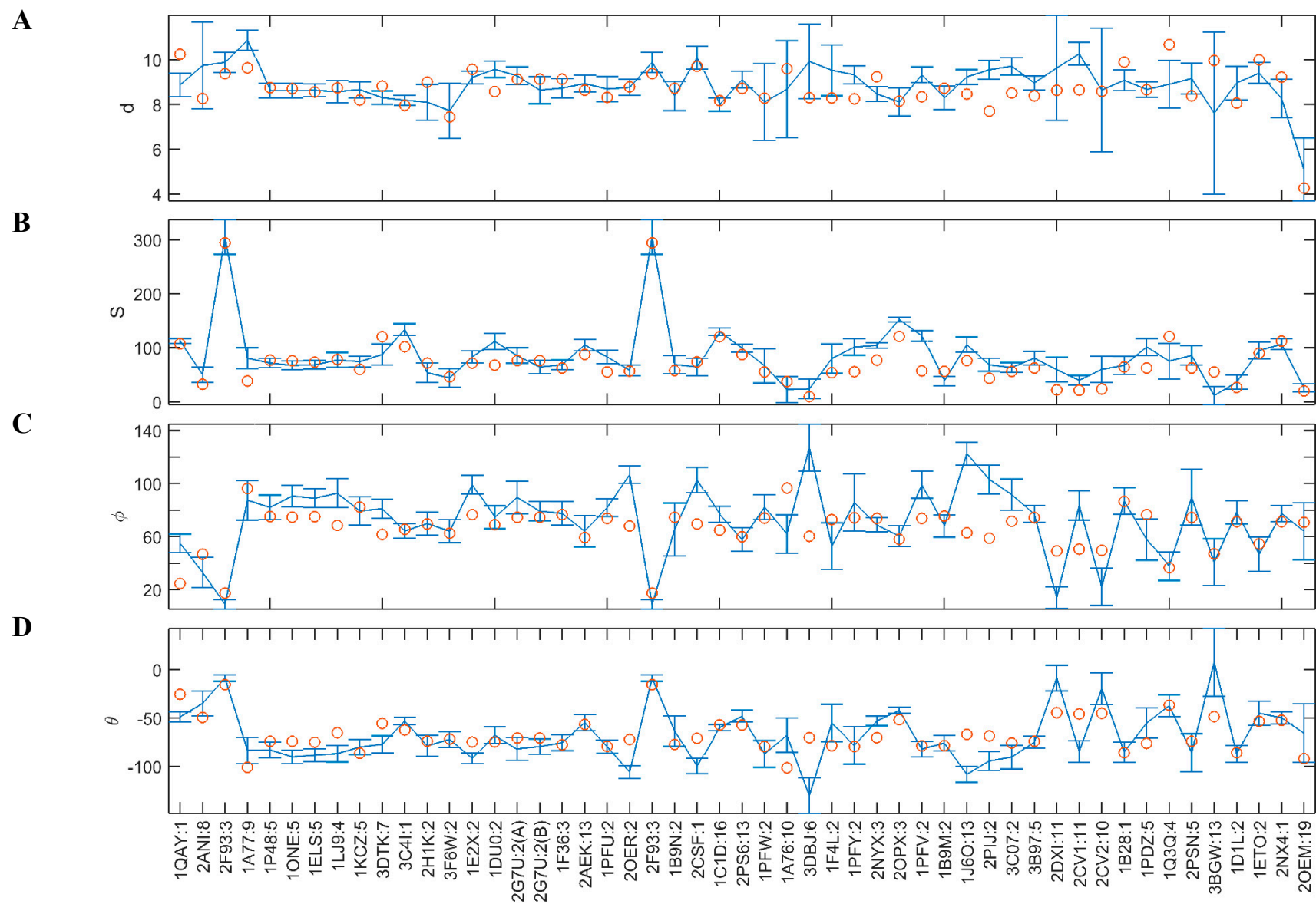
A: interplanar distance (d) between the helices;

B: areas (S) of intersection for the helical projections;

C and D show the φ and θ angles between the helical axes of the structural motif, respectively.

The OX axis represents PDB IDs of the structures, the OY axis represents the values of the studied characteristics: initial value (red circle), average value during the MD experiment (blue point), and standard deviation

For each corner, the red circle marks the values for the characteristics calculated before the start of the experiment, and presents the average value of this characteristic during the MD experiment and its root-mean-square deviation. For the most stable structures, the initial value is as close as possible to the mean and within the interval (mean value \pm standard deviation). This position is desirable for all investigated geometric characteristics of corners. The figure shows that this is not always the case. However, even if some characteristics present less stability, others were stable during the experiment, which helps to maintain the stability of the entire structure.



Results of the MD experiment

Table S1. The results of calculating the geometric characteristics of the structural blocks of protein molecules using the molecular dynamics experiment.

PDB ID	Charge structure	$d, \text{\AA}$	$\bar{d} \text{\AA}$	$\sigma(\bar{d})$	$S, \text{\AA}^2$	$\bar{S} \text{\AA}^2$	$\sigma(\bar{S})$	φ	$\bar{\varphi}$	$\sigma(\bar{\varphi})$	θ	$\bar{\theta}$	$\sigma(\bar{\theta})$
1QAY: 1	q = -1	10,24	8,87	0,53	107,41	112,68	4,58	24,5	54,96	6,96	-25,43	-48,76	5,04
2ANI: 8	q = -3	8,26	9,74	1,93	32,7	50,47	14,22	46,75	33,02	11,39	-49,38	-34,92	12,83
2F93 : 3	q = 0	9,38	9,88	0,45	294,49	304,89	31,8	17,38	8,88	3,68	-15,44	-8,55	3,43
1A77 : 9	q = -4	9,63	10,87	0,45	38,59	80,77	19,21	96,35	87,38	14,9	-100,87	-83,39	13,67
1P48 : 5	q = 2	8,75	8,62	0,33	77,29	71,74	8,66	75,07	82,02	9,26	-74,07	-82,91	8,27
1ONE :5	q = 2	8,7	8,61	0,33	75,84	67,5	7,92	74,6	90,56	8,22	-73,95	-90,09	6,91
1ELS : 5	q = 2	8,56	8,63	0,29	73,22	68,42	7,94	74,99	88,92	7,1	-74,85	-88,33	6,6
1LJ9 : 4	q = 2	8,74	8,57	0,5	78,16	77,4	13,79	68,37	92,72	10,85	-65,12	-86,74	8,51
1KCZ : 5	q = 2	8,2	8,66	0,36	59,89	74,39	9,95	82,24	79,36	10,72	-86,31	-80,02	7,7
3DTK :7	q = 2	8,82	8,3	0,3	120,45	87,55	19,6	61,6	80,98	7,23	-55,53	-77,16	8,9
3C4I : 1	q = 1	7,96	8,19	0,22	101,89	133,88	10,6	65,54	64,23	5,44	-62,23	-53	3,78
2H1K : 2	q = 7	9	8,1	0,8	71,86	53,89	17,79	69,54	69,85	8,71	-73,9	-78,68	10,98
3F6W : 2	q = 3	7,44	7,72	1,23	46,1	44,38	17,07	62,5	64,06	8,71	-71,67	-72,07	8,13
1E2X : 2	q = 2	9,57	9,21	0,29	71,73	83,15	10,96	76,51	99,05	7,04	-74,73	-91,65	5,42
1DU0 : 2	q = 5	8,57	9,57	0,37	68,14	111,79	14,82	68,89	74,54	8,63	-74,6	-67,63	8,6
2G7U:(A):2	q = 3	9,13	9,28	0,4	76,2	85,52	14,3	74,47	89,54	12,37	-70,67	-81,89	11,73
2G7U:(B):2	q = 3	9,13	8,64	0,61	76,2	64,52	12,34	74,47	79,22	7,26	-70,67	-79,48	7,84
1F36 : 3	q = 7	9,13	8,73	0,43	62,78	68,47	9,16	76,52	77,43	8,84	-77,67	-75,51	8,05
2AEK:13	q = -1	8,64	8,93	0,37	87,77	105,21	10,52	59,24	64,09	11,82	-56,54	-54,58	8,33
1PFU : 2	q = -2	8,32	8,69	0,57	55,52	83,16	12,38	73,79	81,88	6,81	-79,09	-79,66	6,64
2OER : 2	q = 2	8,79	8,76	0,36	57,03	58,43	9,87	67,93	106,74	6,49	-72,04	-105,77	6,63
2F93 : 3	q = 0	9,38	9,88	0,45	294,49	304,89	31,8	17,38	8,88	3,68	-15,44	-8,55	3,43
1B9N : 2	q = 0	8,72	8,38	0,65	57,98	69,1	16,59	74,49	65,28	19,96	-77,31	-63,45	15,86
2CSF : 1	q = 2	9,71	10,1	0,52	73,93	64,61	15,94	69,54	102,6	9,62	-70,75	-99,54	7,78
1C1D:16	q = -2	8,17	7,99	0,29	120,66	129,82	6,79	64,91	76,8	5,98	-56,98	-59,76	3,3
2PS6 :13	q = -1	8,71	9,11	0,38	87,48	99,48	7,39	59,88	57,67	8,87	-57,16	-48,03	6,1
1PFW : 2	q = -2	8,28	8,11	1,72	55,47	66,75	31,37	73,85	82,25	9,22	-79,34	-87	13,89
1A76 :10	q = -4	9,6	8,68	2,17	37,47	22,77	23,99	96,62	62,07	14,54	-101,32	-67,76	17,71
3DBJ : 6	q = 2	8,3	9,92	1,67	10,17	24,16	18,36	60,22	127,15	17,73	-70,2	-130,15	18,55
1F4L : 2	q = -2	8,29	9,53	1,14	53,97	80,06	27,18	72,82	52,82	17,65	-78,52	-55,11	19,37
1PFY : 2	q = -2	8,25	9,32	0,4	55,74	101,25	15,09	74,25	85,7	21,66	-79,32	-78,18	19,39
2NYX: 3	q = 2	9,24	8,47	0,33	77,03	104,49	4,87	73,69	68,77	5,38	-70,28	-52,95	4,99
2OPX : 3	q = -4	8,14	8,11	0,62	120,91	151,94	4,28	57,94	60,4	7,77	-51,69	-42,04	3,25
1PFV : 2	q = -2	8,34	9,33	0,35	57,23	122,12	9,94	73,74	99,02	10,26	-78,66	-82,1	8,03
1B9M : 2	q = 0	8,72	8,29	0,53	56,59	38,76	8,81	75,38	67,85	8,39	-78,47	-75,89	8,05
1J6O :13	q = 0	8,46	9,23	0,33	76,26	105,86	13,89	62,85	122,64	8,52	-66,88	-108,13	8,1

2PIJ : 2	q = 2	7,7	9,55	0,42	43,54	68,45	11,99	58,8	103,19	10,89	-68,52	-94,33	9,76
3C07 : 2	q = 1	8,51	9,71	0,39	56,16	63,49	9,17	71,58	91,64	11,88	-75,69	-90,22	12,19
3B97 : 5	q = 2	8,38	8,96	0,31	62,82	80,88	12,61	74,35	76,98	6,44	-74,13	-75	6,26
2DXI : 11	q = 0	8,63	9,63	2,35	22,23	59,58	22,72	49,11	13,94	8,26	-44,35	-8,59	13,29
2CV1 : 11	q = 0	8,65	10,26	0,51	21,68	39,91	8,84	50,47	83,48	11,03	-45,68	-84,58	11,09
2CV2 : 10	q = 0	8,58	8,64	2,77	23,71	60,06	24,5	49,64	22,07	14,01	-45,15	-19,55	16,25
1B28 : 1	q = 0	9,89	9,08	0,47	64,63	67,45	16,5	86,56	86,82	10,14	-85,69	-85,11	10,41
1PDZ : 5	q = 2	8,66	8,67	0,34	62,63	101,54	15,64	76,53	57,84	15,65	-76,21	-54,99	15,43
1Q3Q : 4	q = -3	10,68	8,9	1,07	121,12	75,4	33	36,49	37,68	10,82	-36,83	-37,21	11,36
2PSN : 5	q = 2	8,38	9,16	0,69	62,83	85,86	17,93	74,29	89,68	21,07	-74,08	-85,78	19,55
3BGW : 13	q = 6	9,97	7,61	3,63	55,22	11,63	16,8	46,91	40,65	17,62	-48,39	7,65	35,05
1D1L : 2	q = 3	8,06	8,96	0,75	26,69	36,52	12,67	71,2	78,29	8,72	-85,8	-87	8,57
1ETO : 2	q = -3	9,99	9,4	0,47	89,94	95,07	15,62	54,44	46,77	12,96	-53,34	-45,06	12,29
2NX4 : 1	q = 2	9,22	8,26	0,86	112,21	106,36	9,89	71,22	77,46	6,04	-52,23	-49,7	6,33

d , S , θ , φ – the values of geometric characteristics calculated before the MD experiment: interplanar distance, area of the polygon of intersection of helical projections, torsion angle between the axes of the helices, two-dimensional angle between the axes of the helices, respectively;

\bar{d} , $\bar{\varphi}$, \bar{S} , $\bar{\theta}$ – average values of the studied quantities during the experiment;

σ – standard deviation.

In order to check the stability of the studied corners for each structural motive (α - α -corner), the following were investigated:

- change in the conformation of the corner constriction. For this, in each of the 5000 frames of the MD experiment, the values of the torsion angles of each amino acid residue of the irregular region were recorded;
- change in the values of the geometric characteristics of the studied motifs during the experiment: the intersection area of the projections of the helixes, the interplanar distance, the angles between the axes of the helixes of the helical pair.

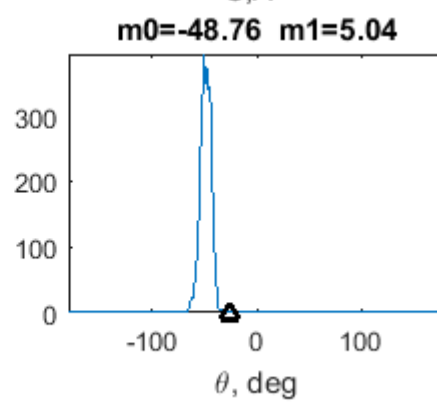
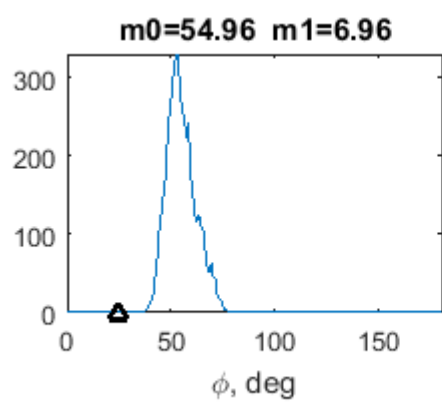
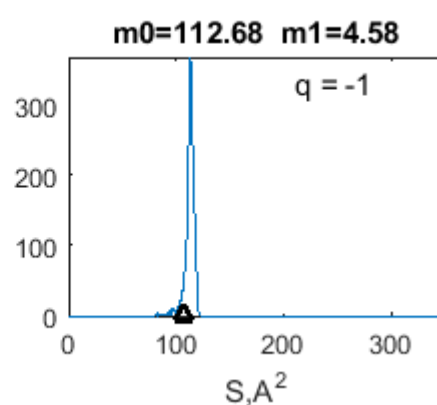
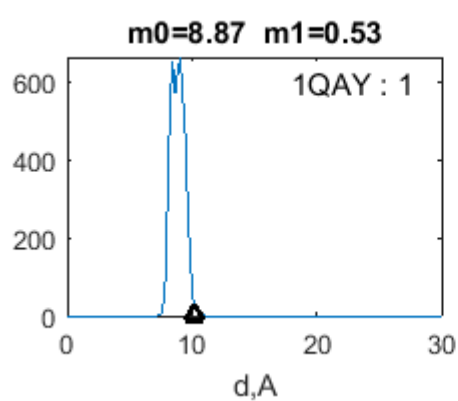
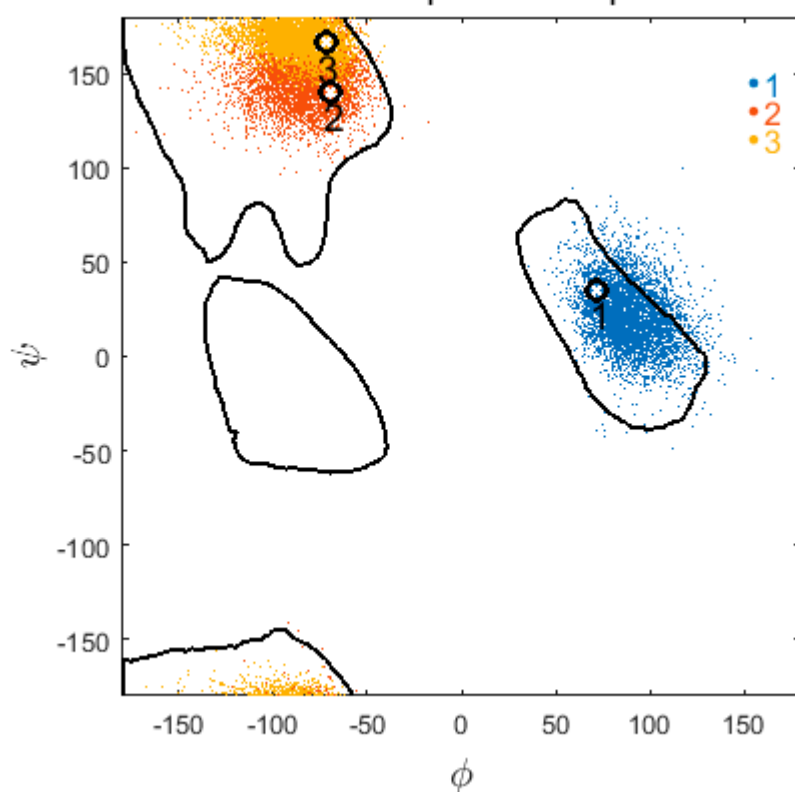
Figures and histograms reflecting these calculations are presented for each structural block.

Each structure is described by two figures:

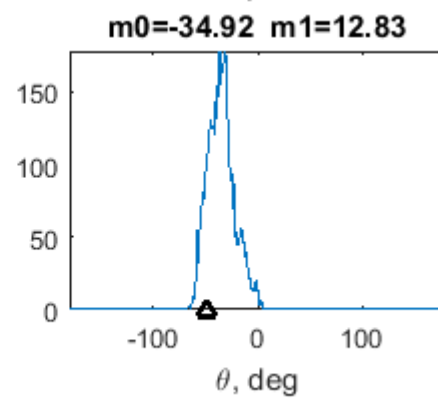
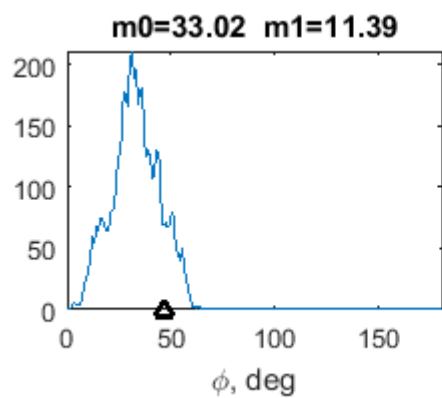
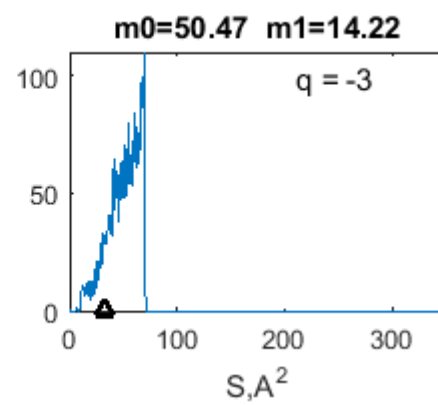
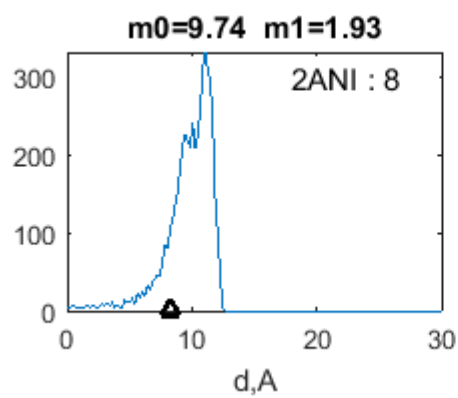
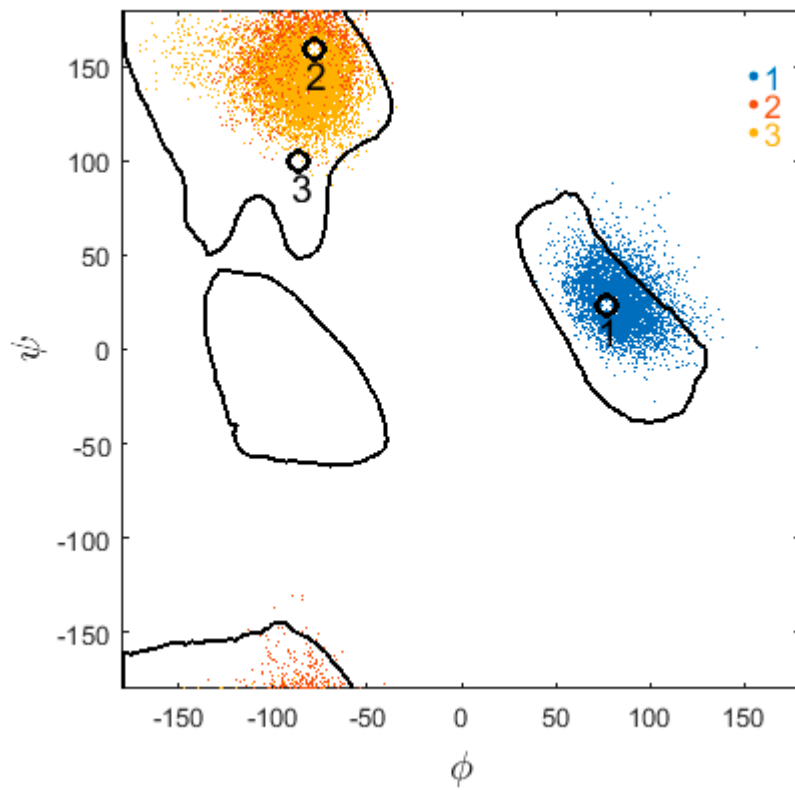
The first figure illustrates the change in the conformation of the constriction of the α - α -corner during the MD experiment by recording the values of the torsion angles φ and ψ of each amino acid residue of the irregular region. The colored dots on the Ramachandran map denote the φ and ψ angles of the constriction amino acids for each point of the trajectory. The legend on the right indicates the sequence of amino acids in the constriction: blue is the first amino acid, red is the second amino acid, orange is the third amino acid, purple is the fourth amino acid, light green is the fifth amino acid, and blue is the sixth amino acid of the constriction. Each point is signed with a serial number, in this sequence are the constriction amino acids of the experimental structure. Black circles are the values of the angles φ and ψ of the experimental structure before the start of the MD experiment. In the caption to Fig. the PDB identifier is given, then the serial number of the helical pair, then two values: ξ_p – the percentage of trajectory points with negative chirality, S_p – the percentage of trajectory points with a nonzero projection area of the helixes.

The second figure is four histograms of quantities describing the geometry of the helical pair (α - α -corner). They illustrate the distributions of the values of geometric characteristics in the course of the MD experiment: the interplanar distance between the helixes, the intersection area of the projections of the helixes, the angles φ and θ between the axes of the helixes of the structural motif. In the captions for each histogram, the mean value m_0 and the standard deviation m_1 . In the figure with the histogram of the interplanar distance, the structure identifier is duplicated, and in the figure with the histogram of the intersection area, the total charge of the structure is shown.

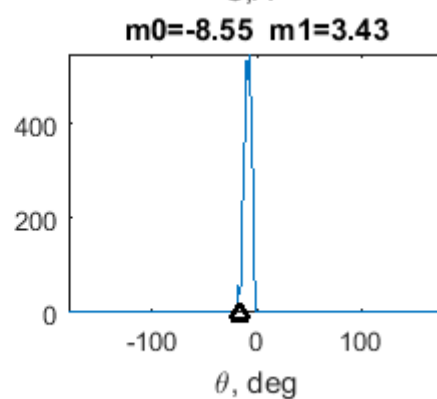
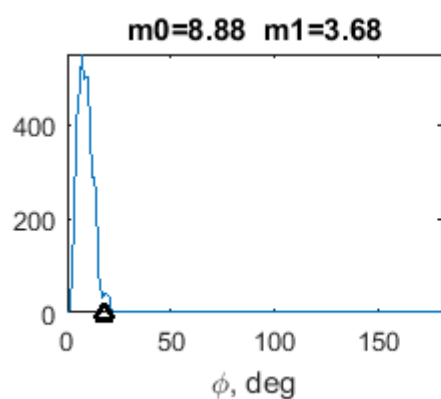
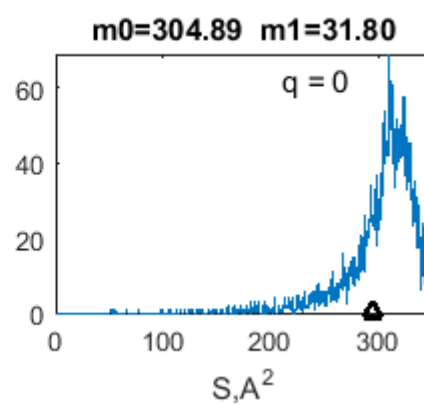
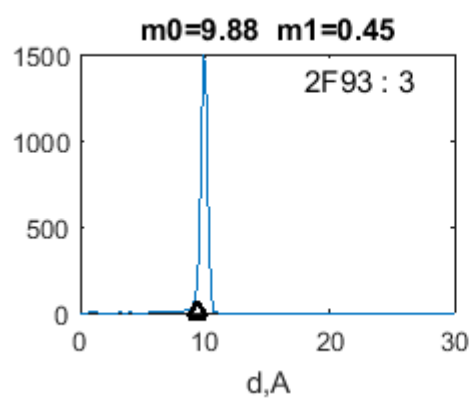
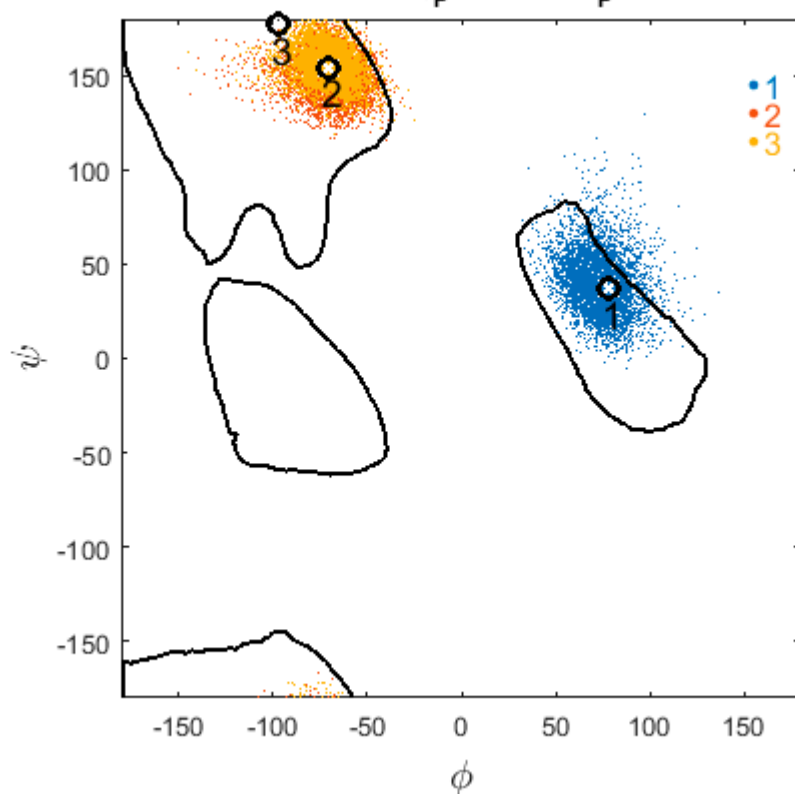
1 1QAY : 1 $\xi_p=100.0\%$ $S_p=100.0\%$



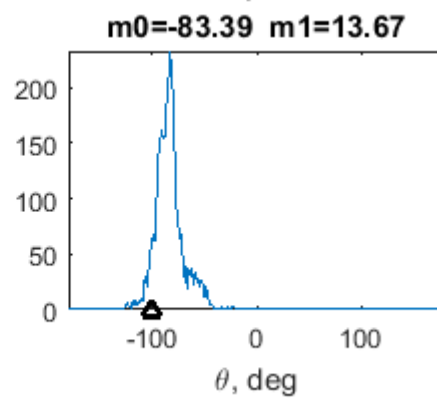
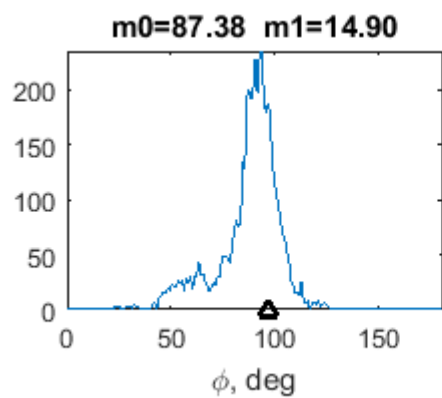
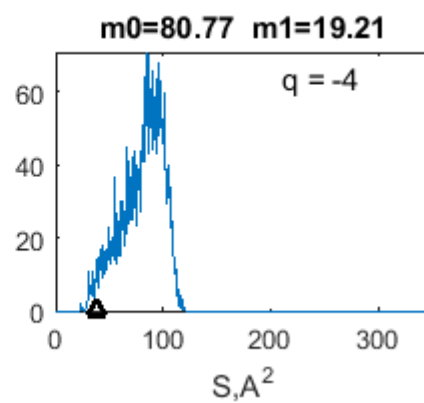
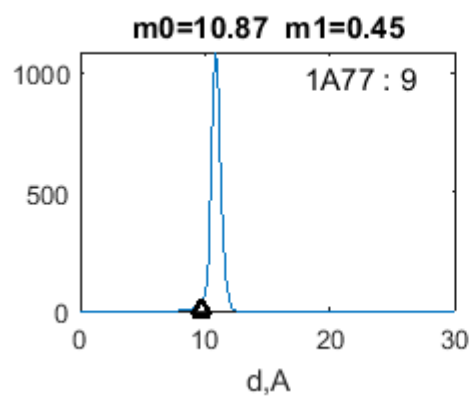
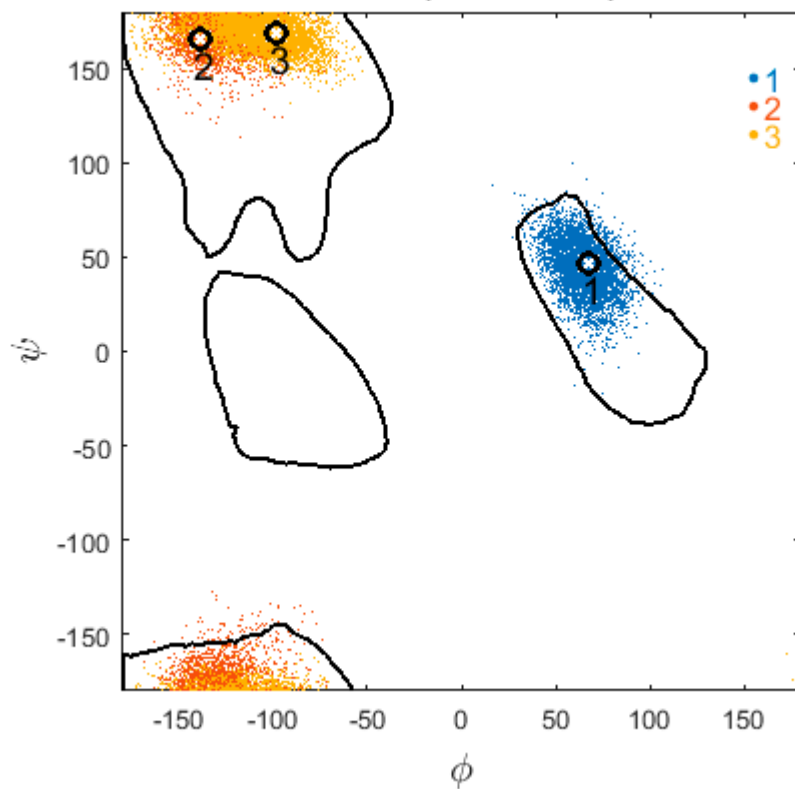
5 2ANI : 8 $\xi_p=99.5\%$ $S_p=100.0\%$



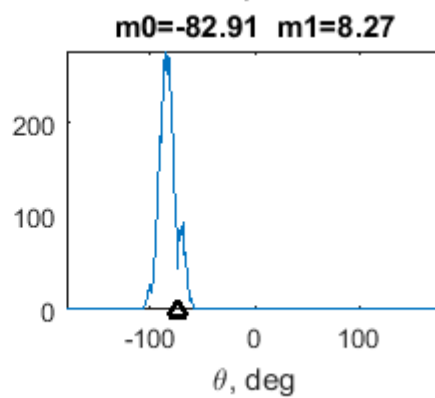
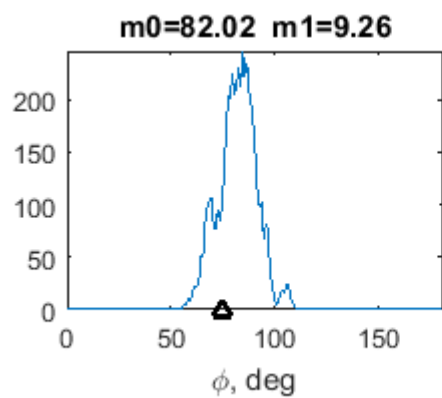
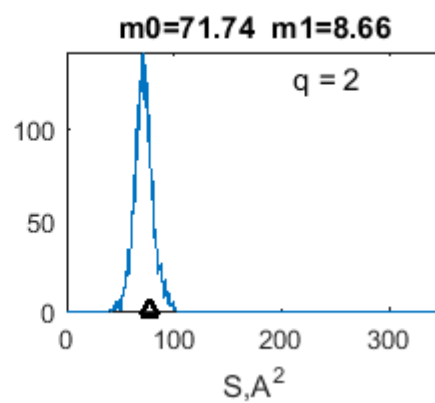
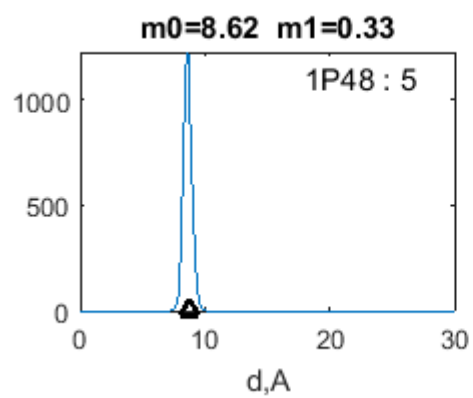
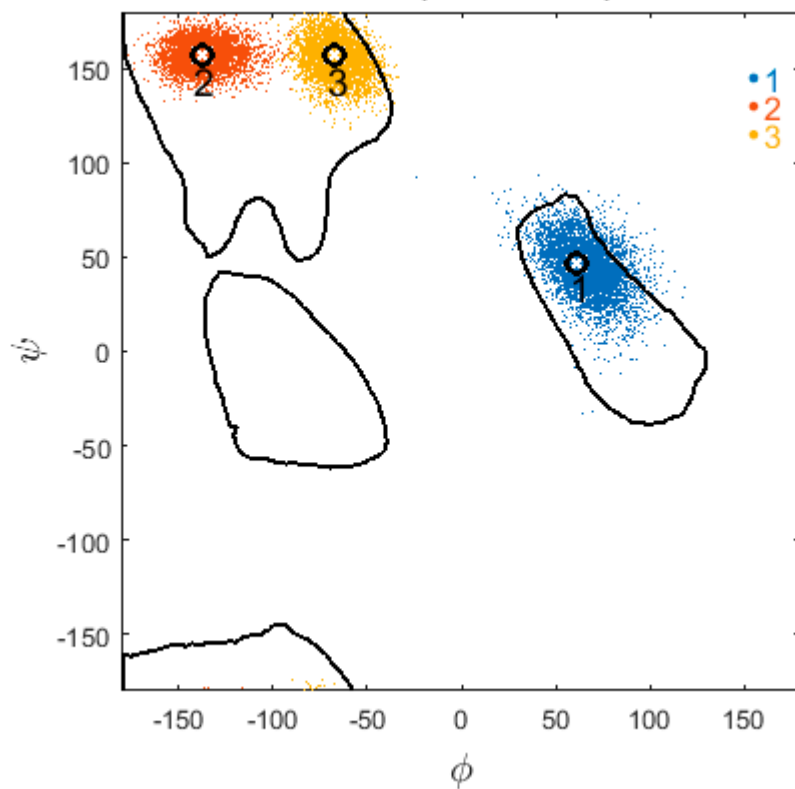
24 2F93 : 3 $\xi_p=99.9\%$ $S_p=100.0\%$



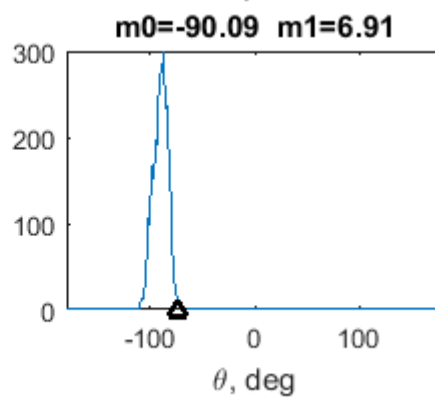
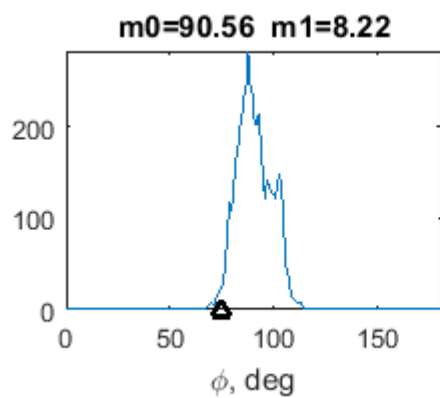
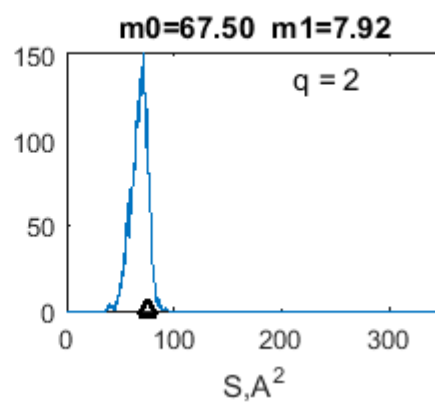
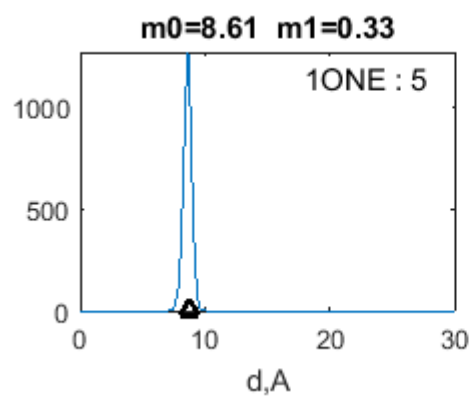
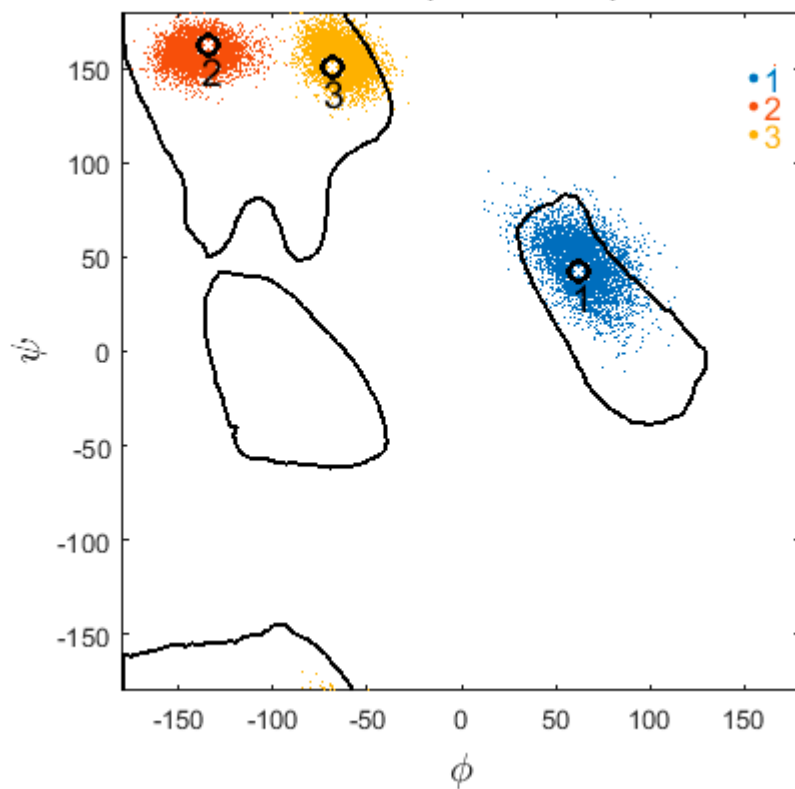
35 1A77 : 9 $\xi_p=100.0\%$ $S_p=100.0\%$



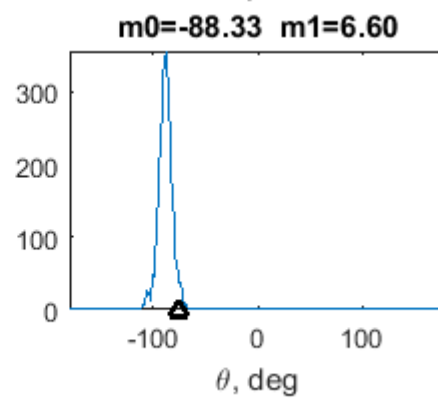
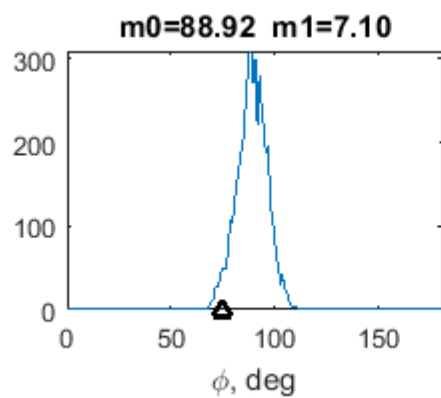
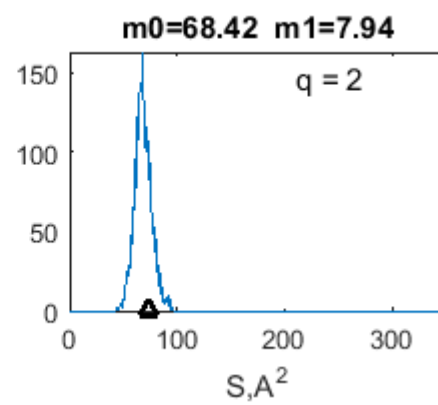
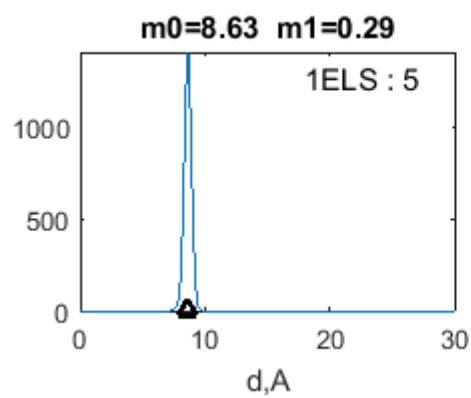
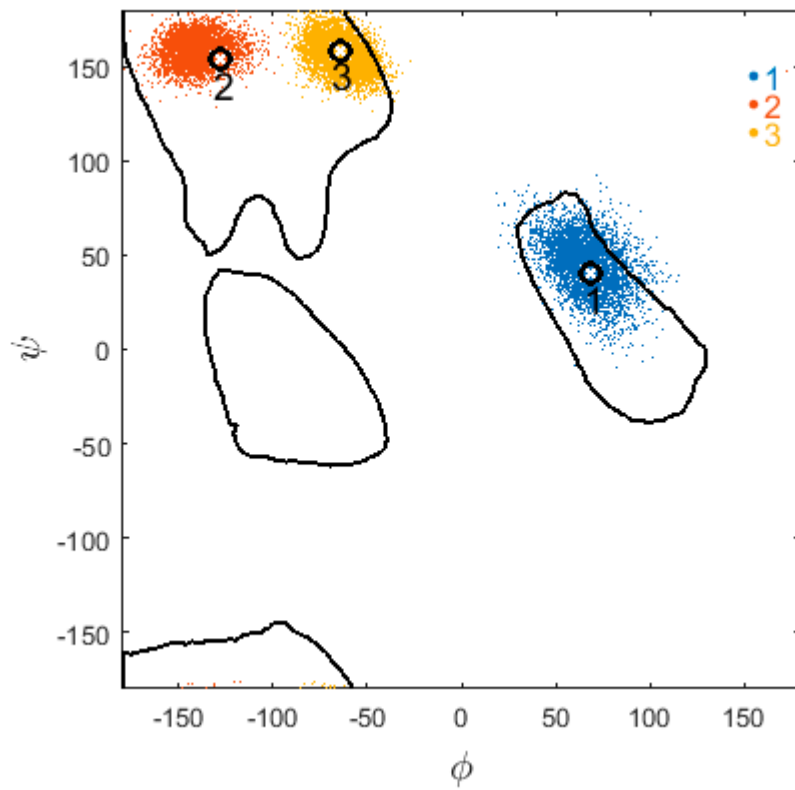
2 1P48 : 5 $\xi_p=100.0\%$ $S_p=100.0\%$



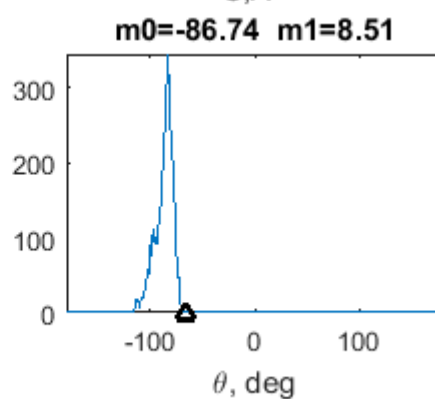
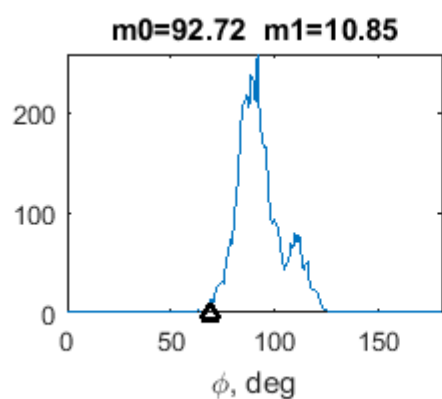
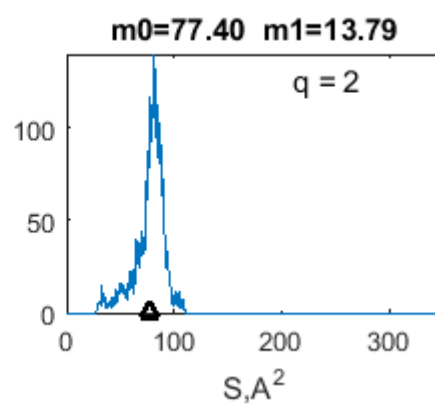
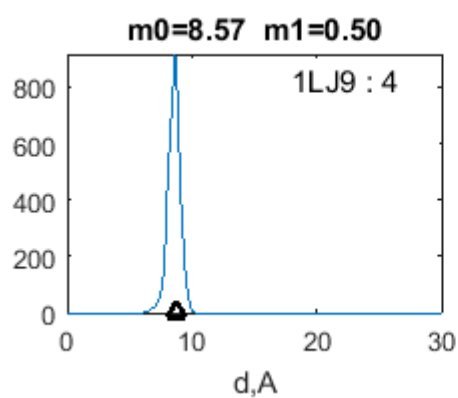
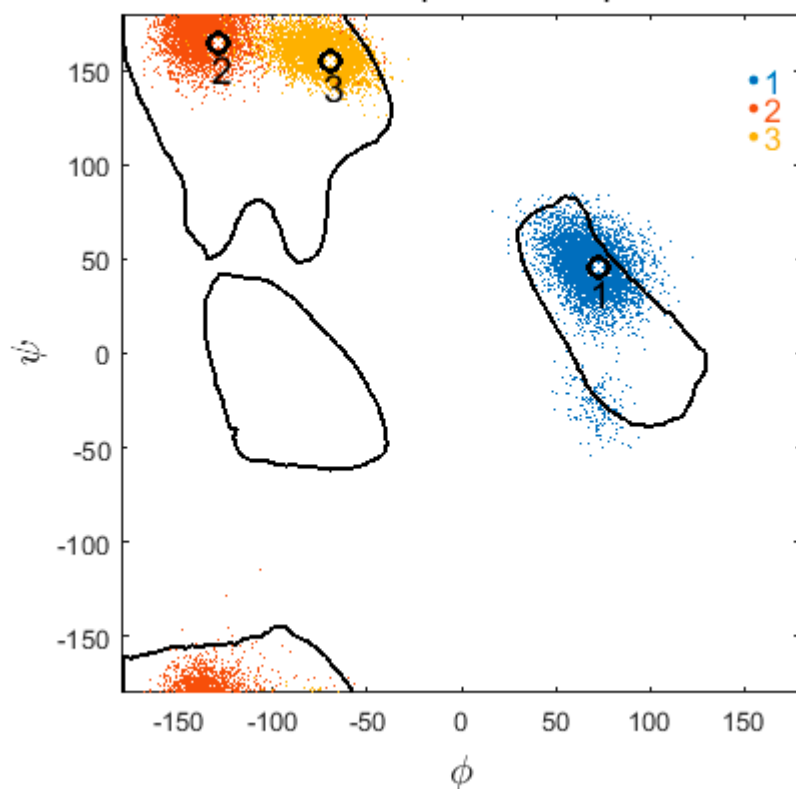
3 1ONE : 5 $\xi_p=100.0\%$ $S_p=100.0\%$

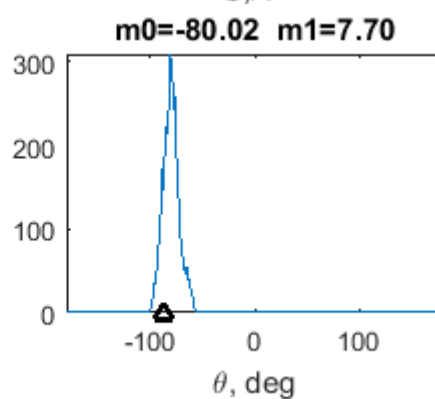
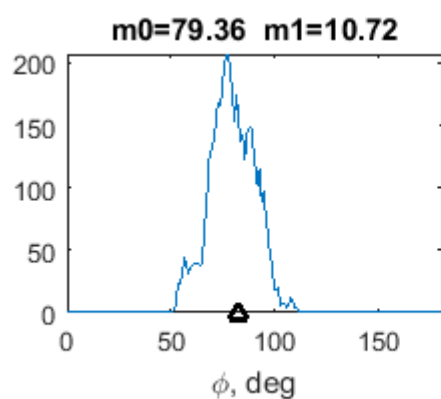
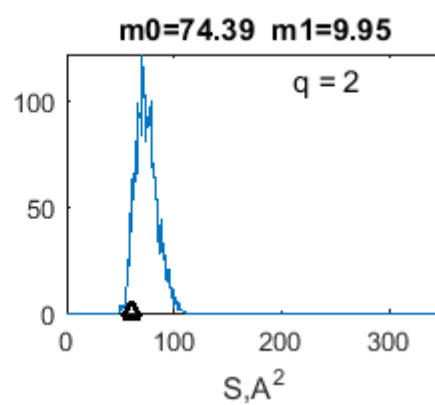
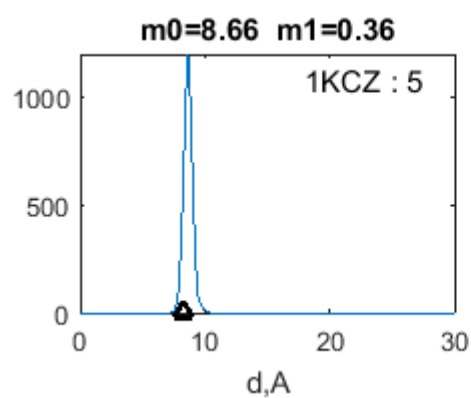
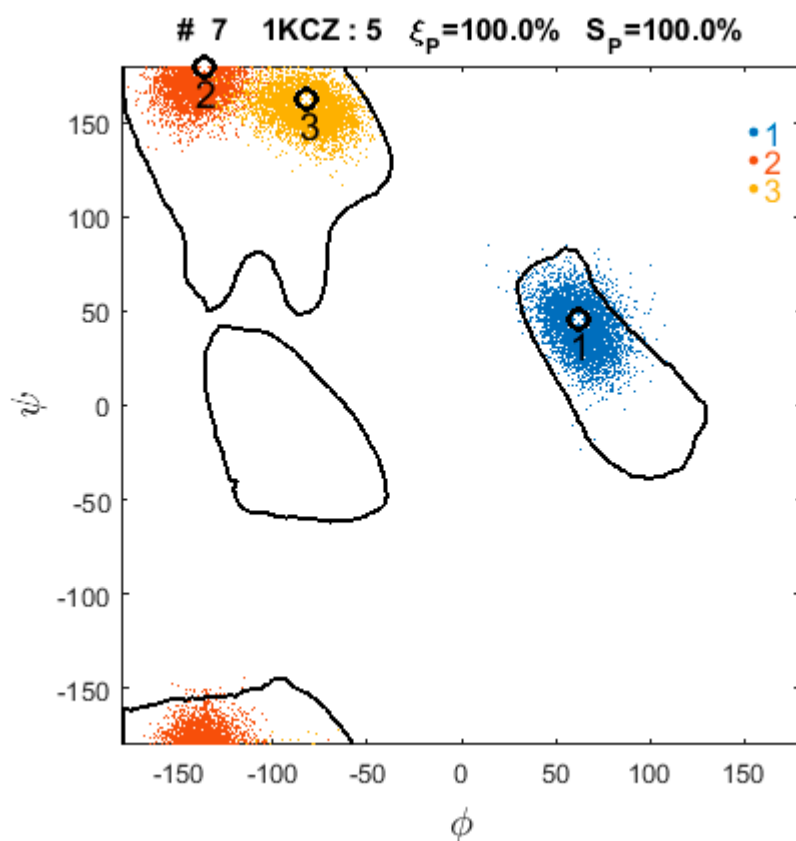


4 1ELS : 5 $\xi_p=100.0\%$ $S_p=100.0\%$

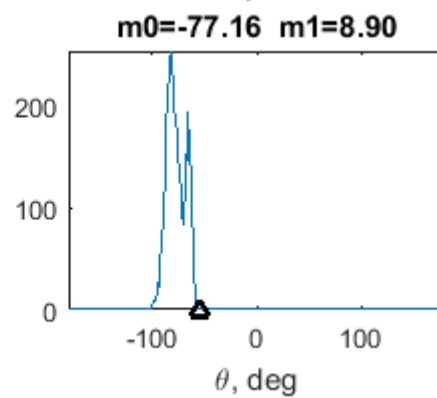
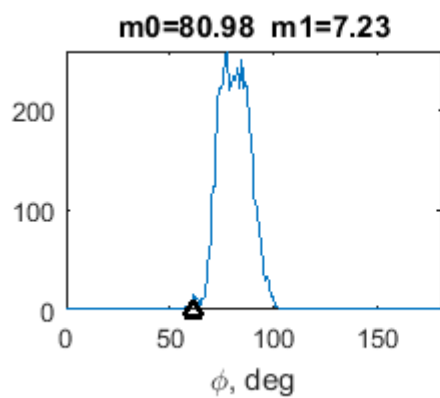
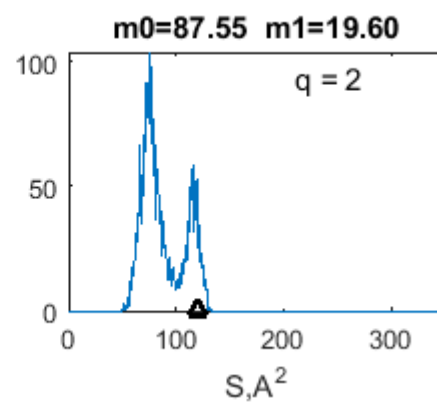
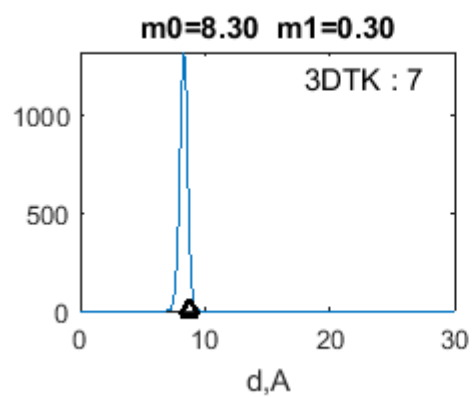
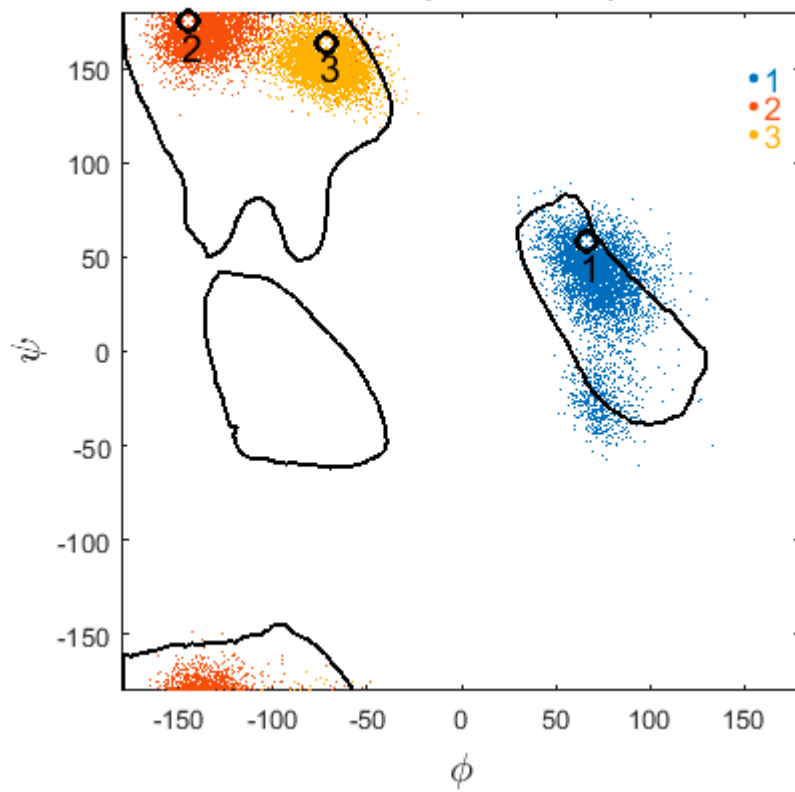


6 1LJ9 : 4 $\xi_p=100.0\%$ $S_p=100.0\%$

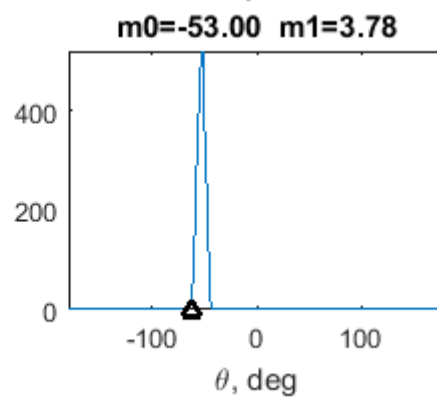
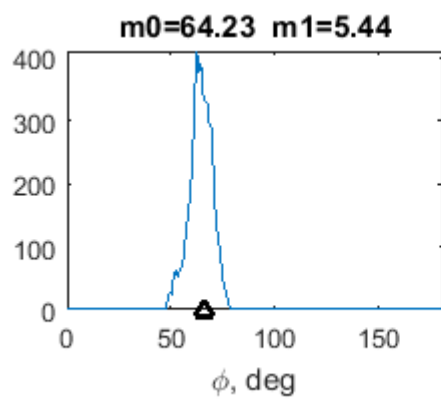
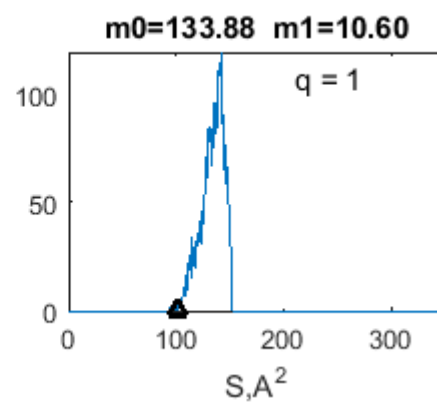
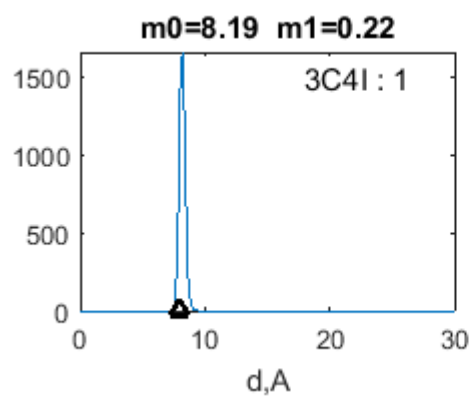
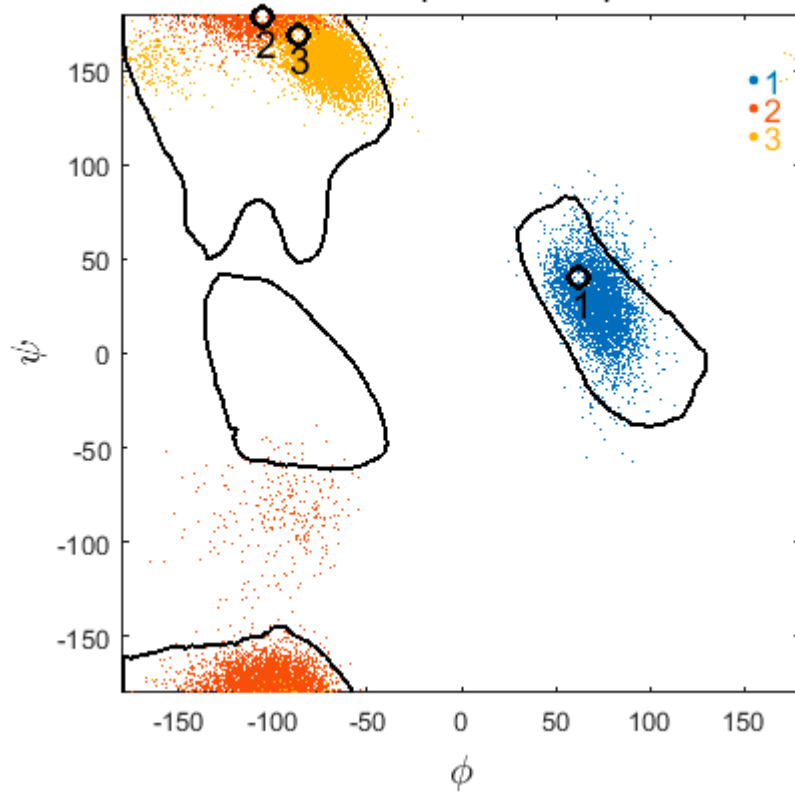




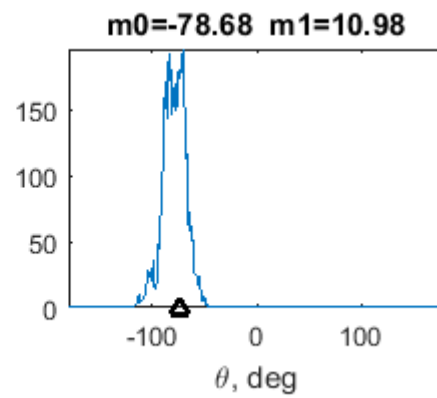
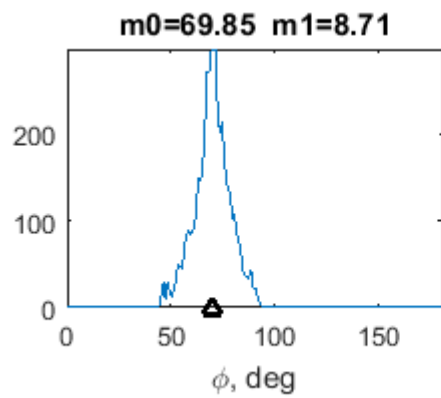
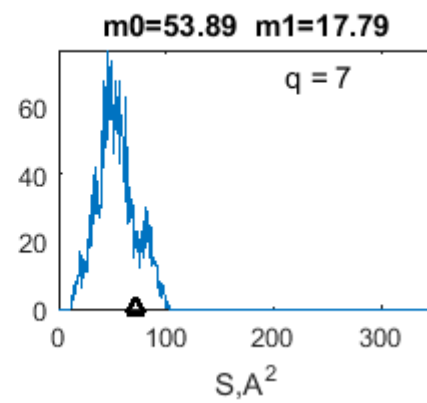
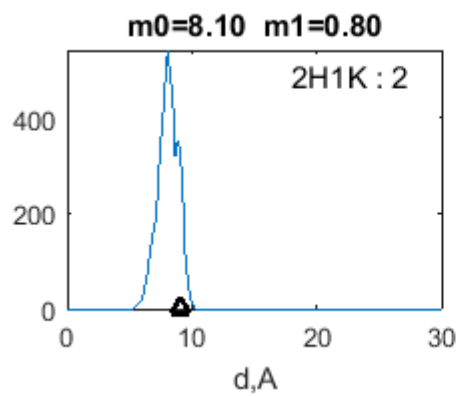
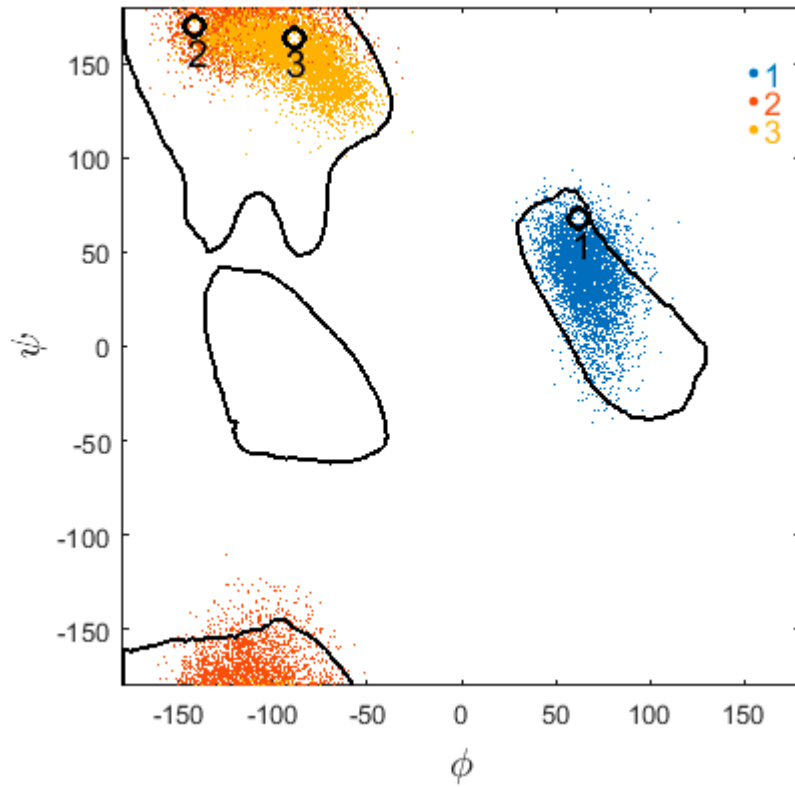
8 3DTK : 7 $\xi_p=100.0\%$ $S_p=100.0\%$



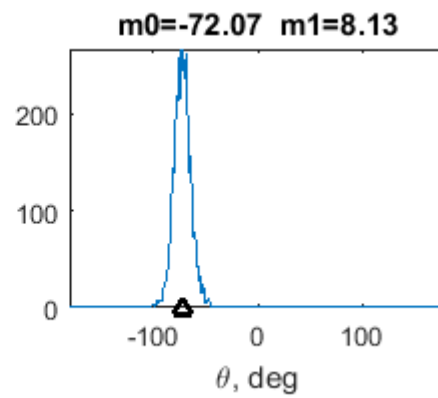
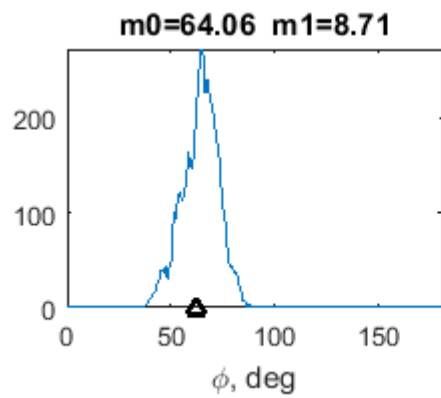
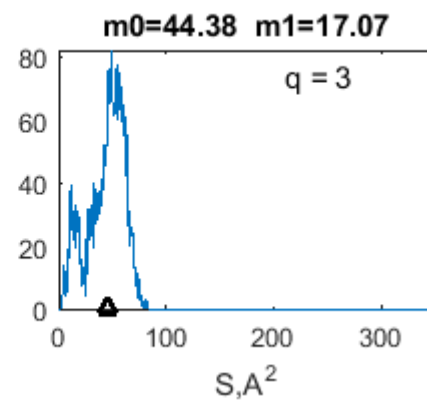
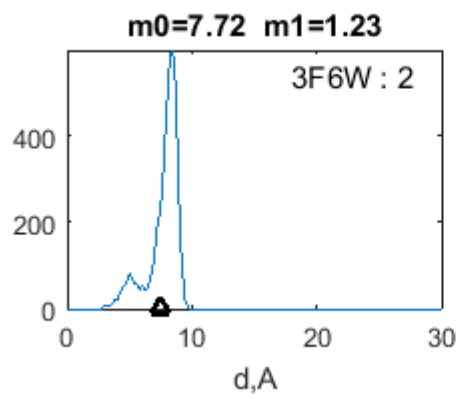
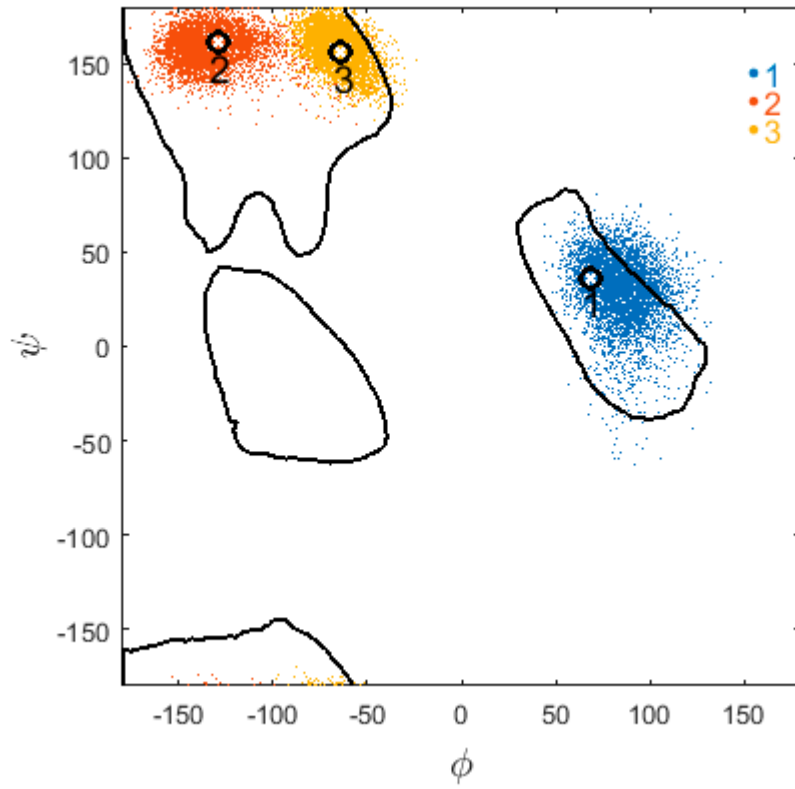
12 3C4I : 1 $\xi_p=100.0\%$ $S_p=100.0\%$



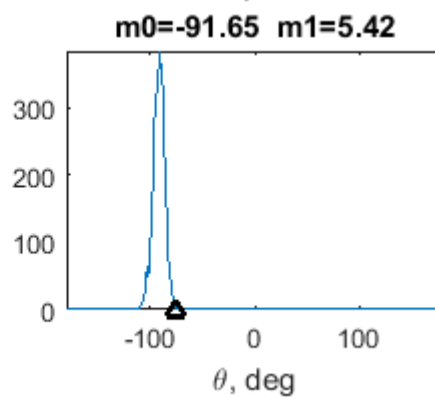
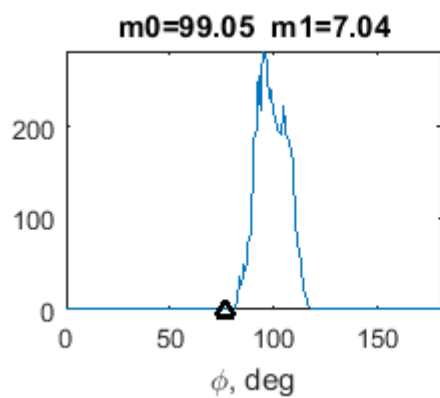
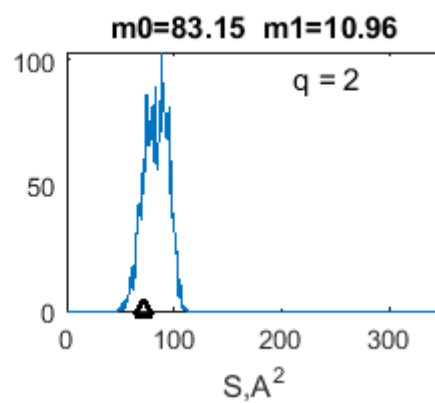
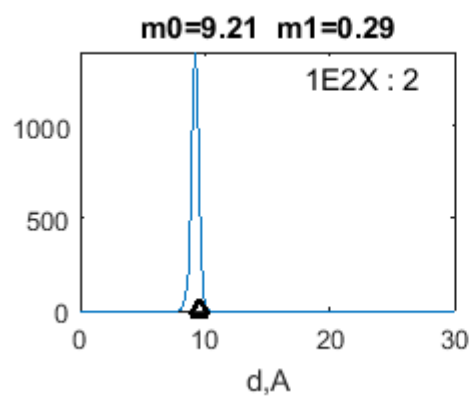
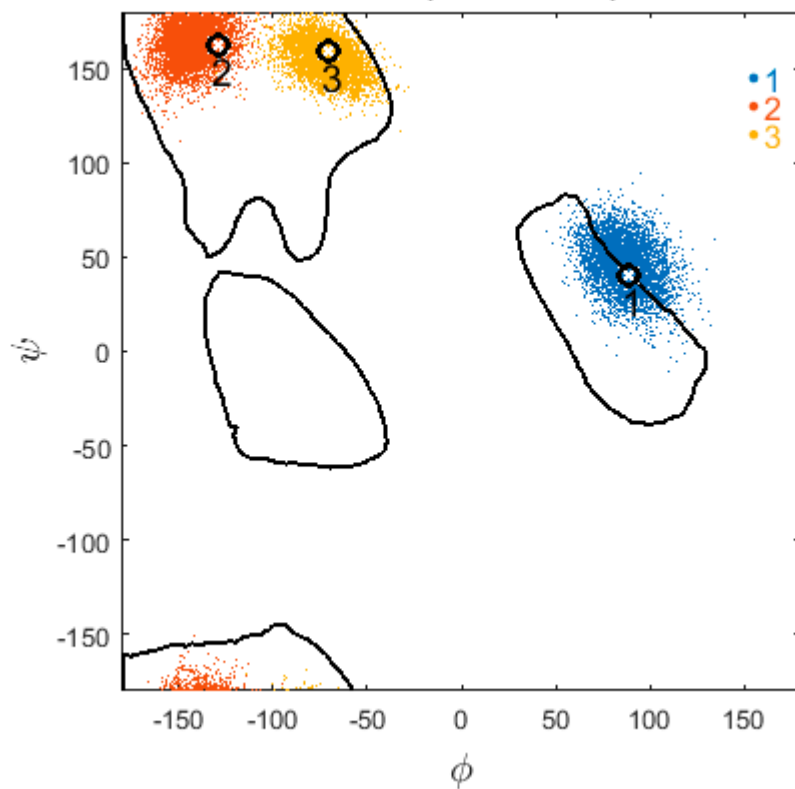
13 2H1K : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



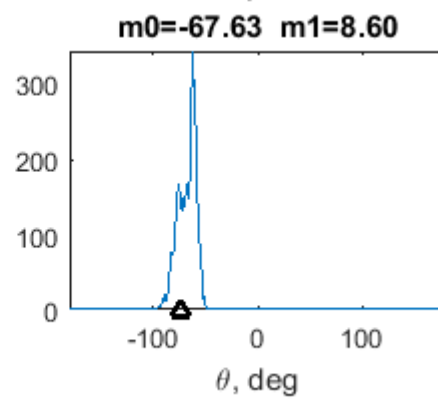
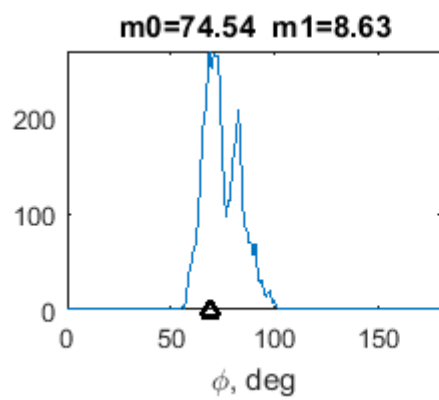
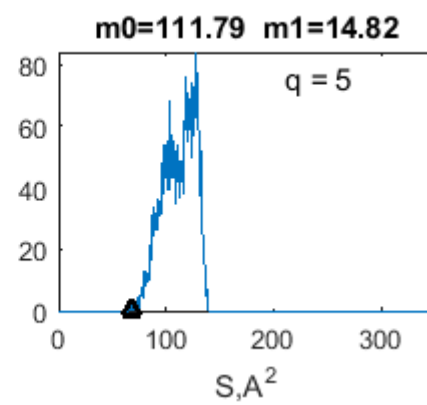
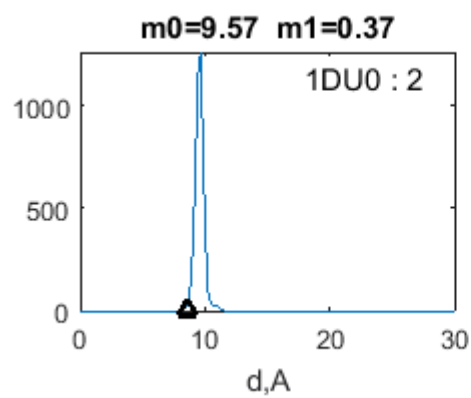
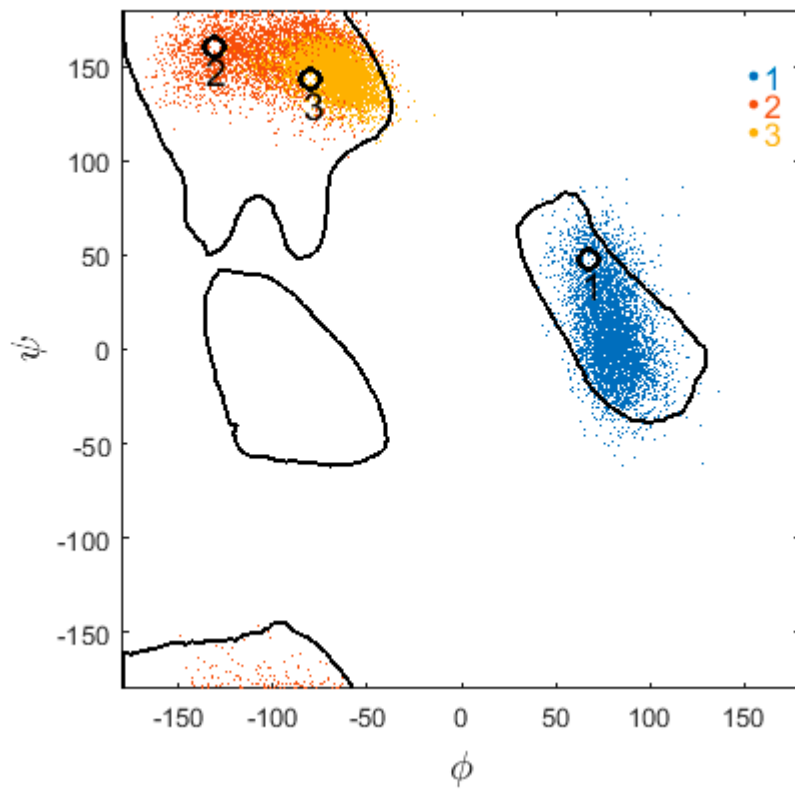
14 3F6W : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



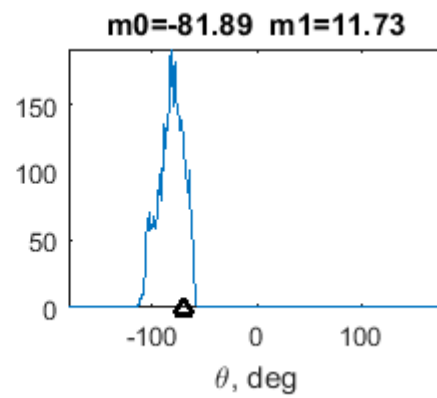
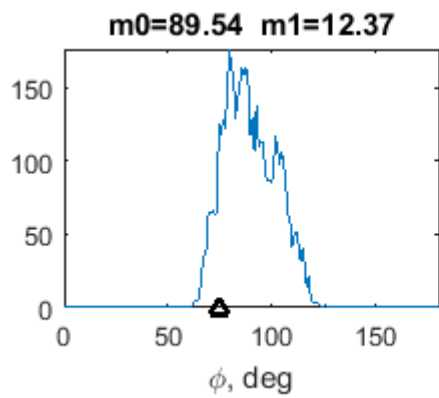
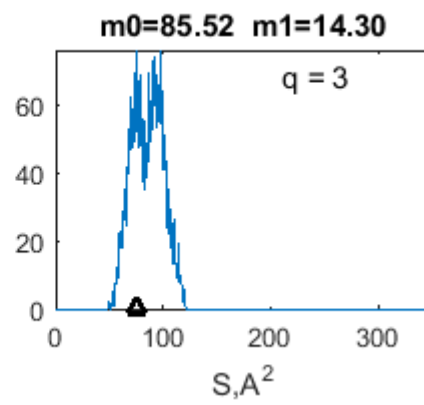
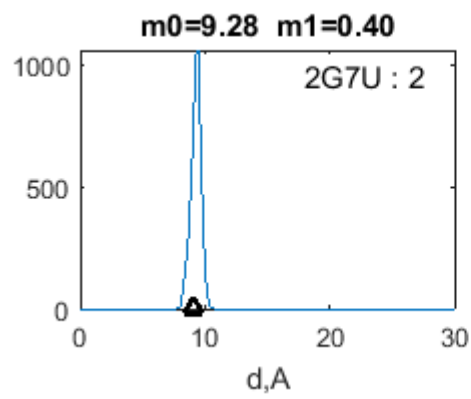
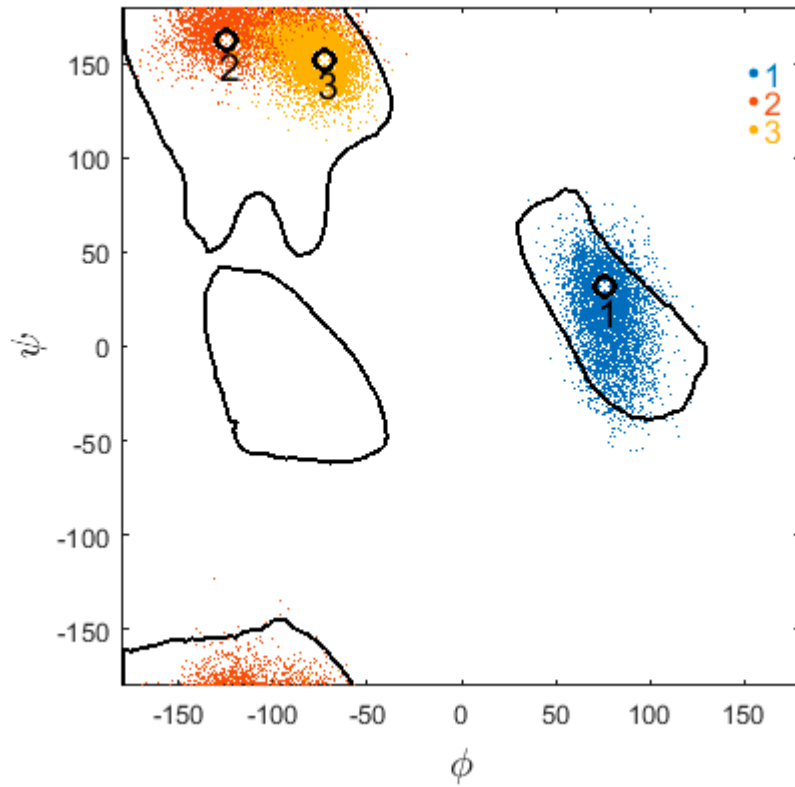
16 1E2X : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



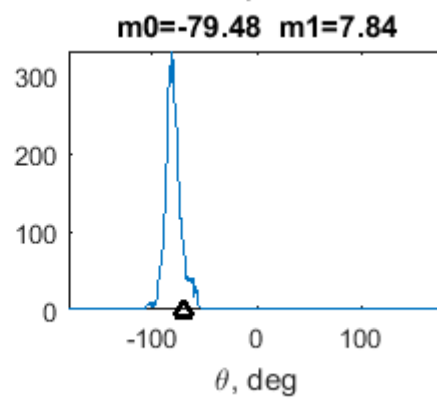
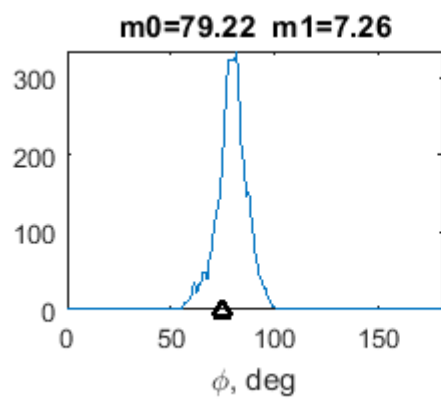
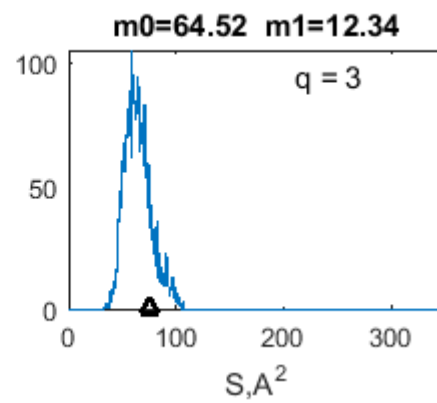
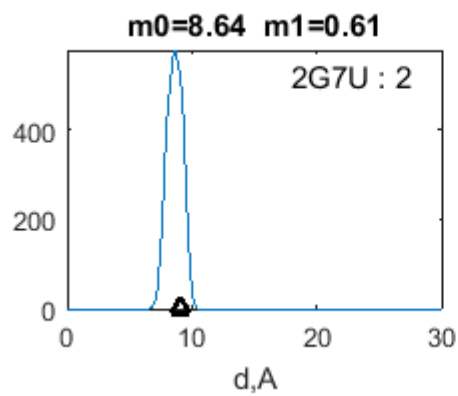
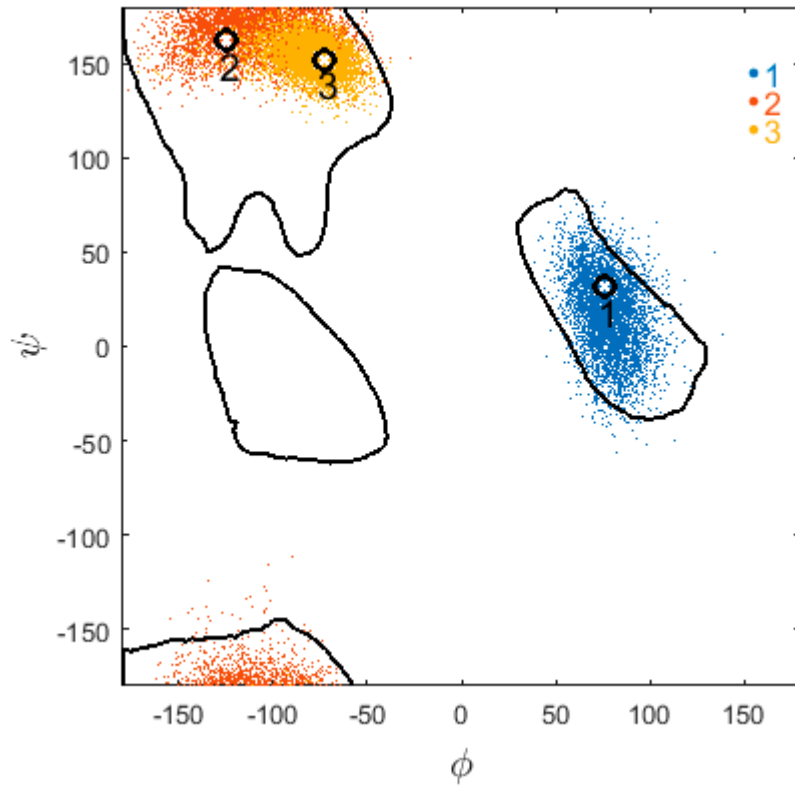
17 1DU0 : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



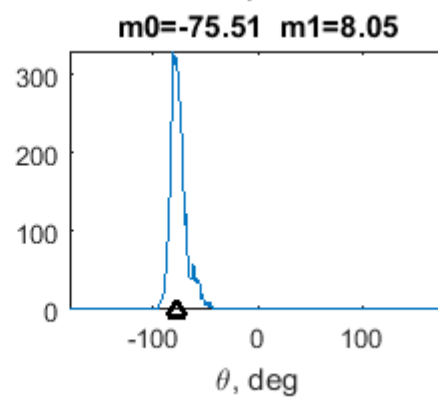
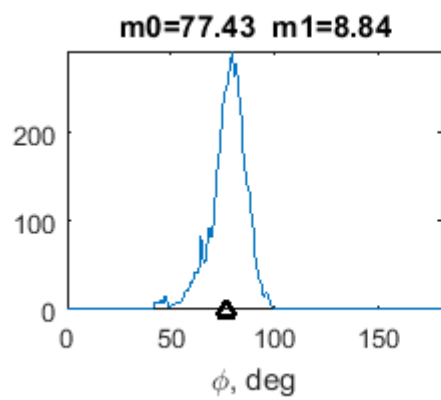
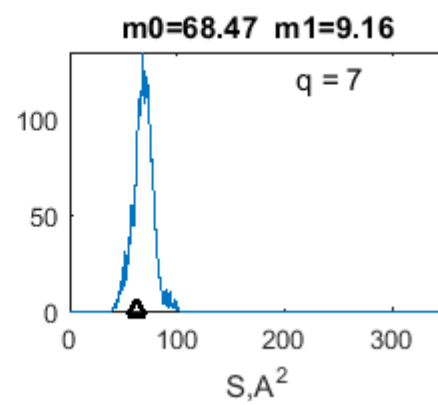
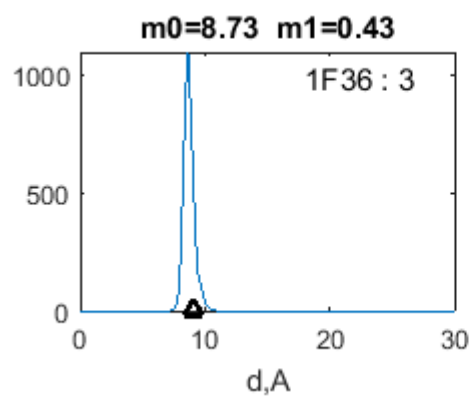
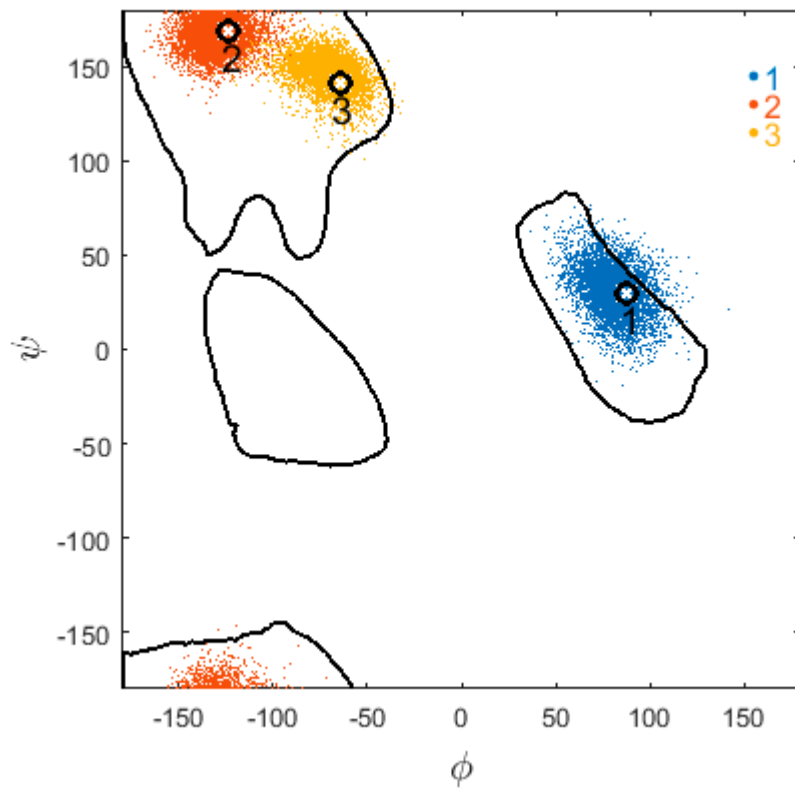
18 2G7U : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



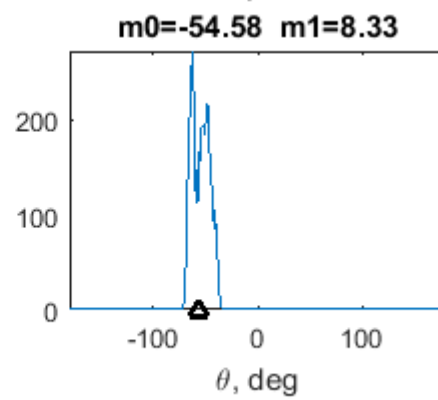
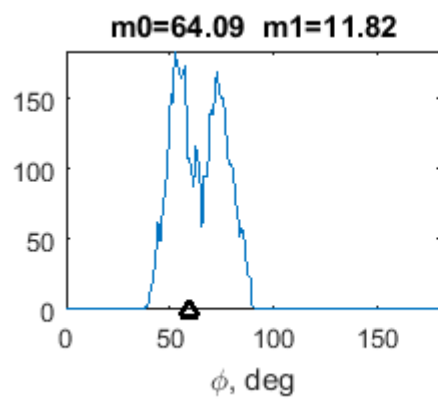
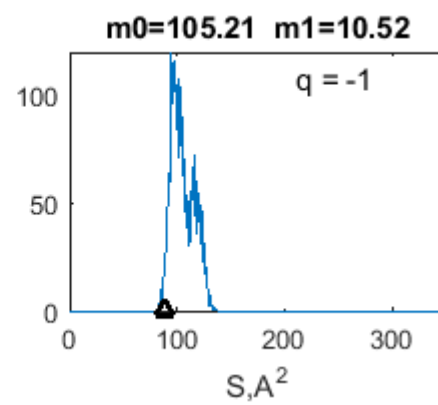
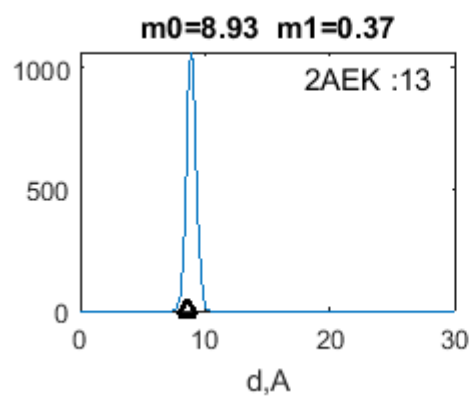
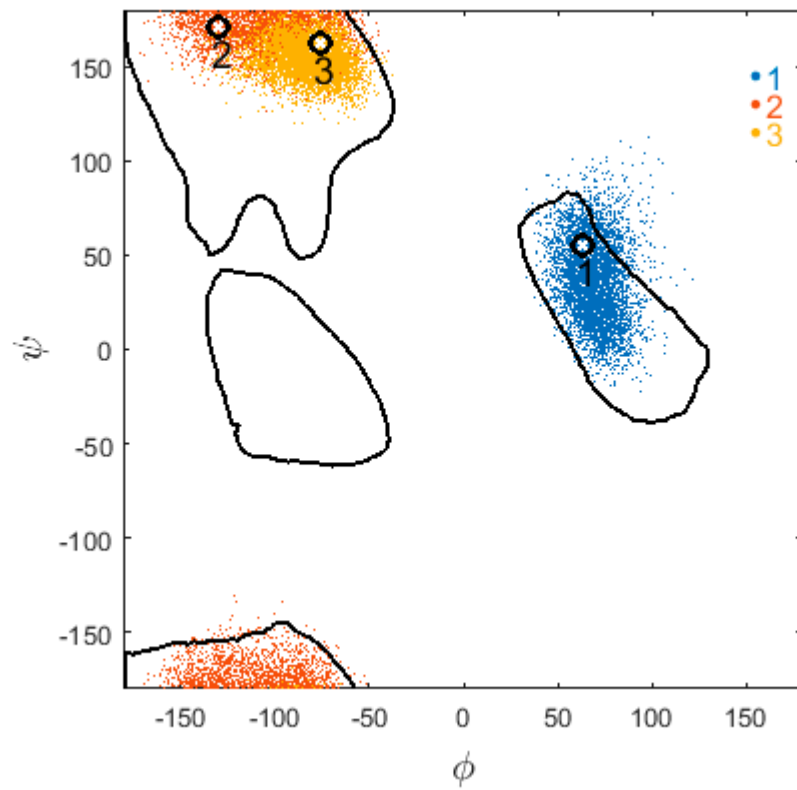
19 2G7U : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



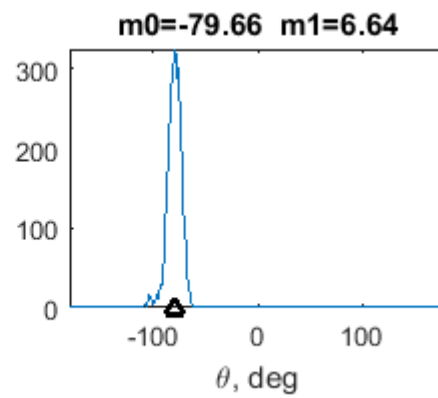
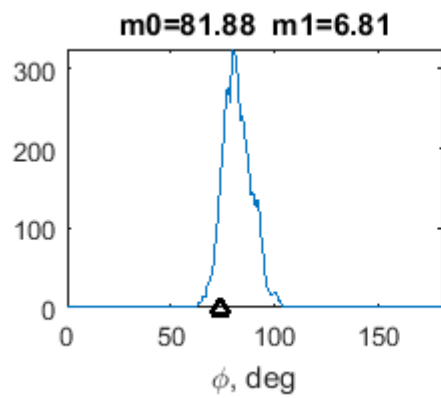
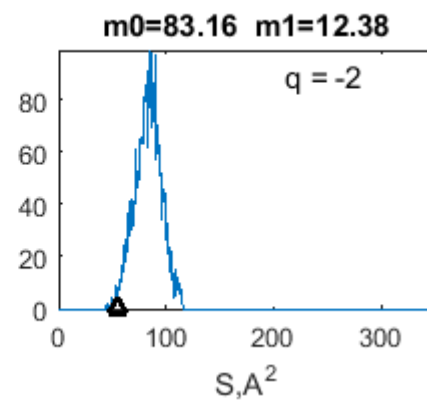
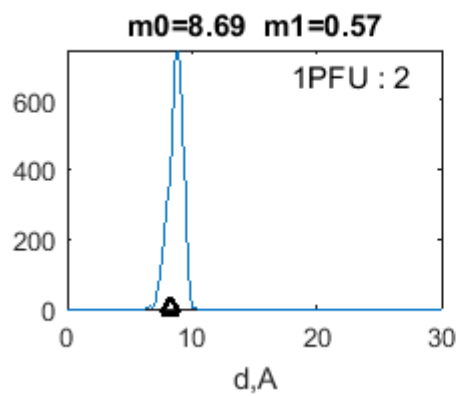
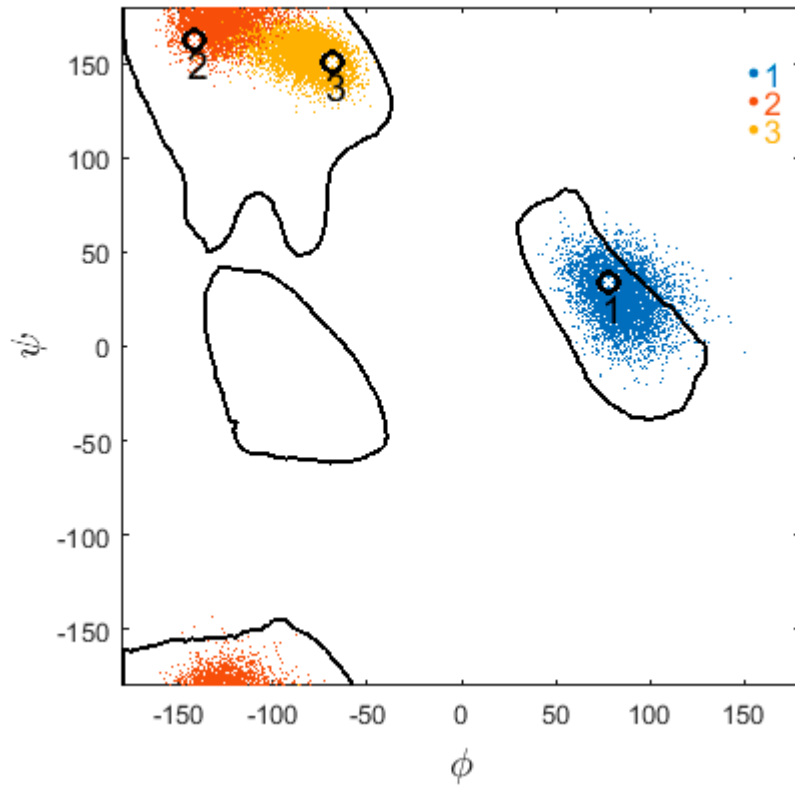
20 1F36 : 3 $\xi_p=100.0\%$ $S_p=100.0\%$



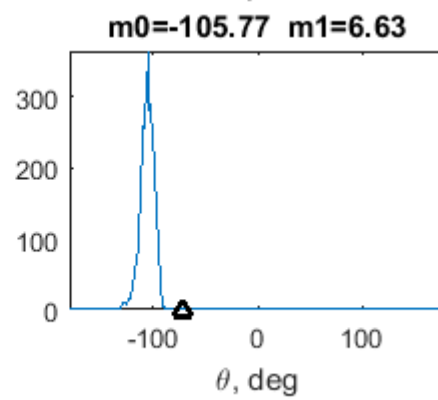
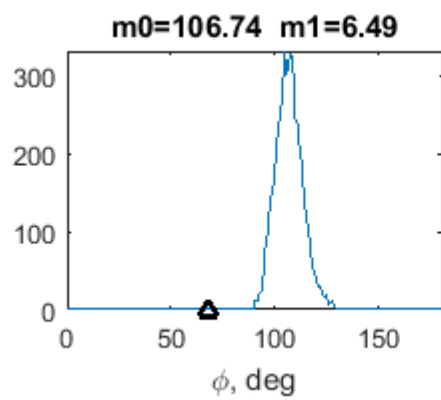
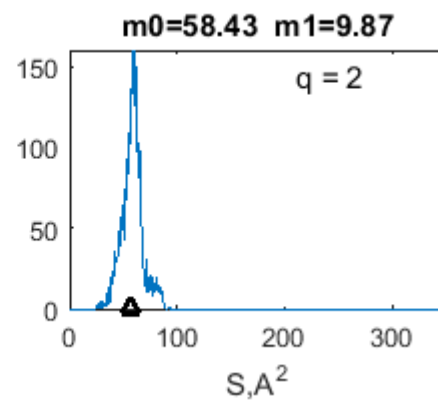
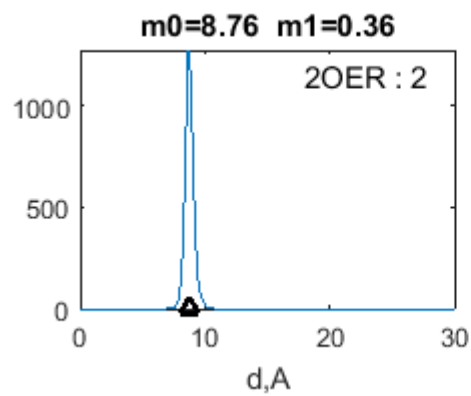
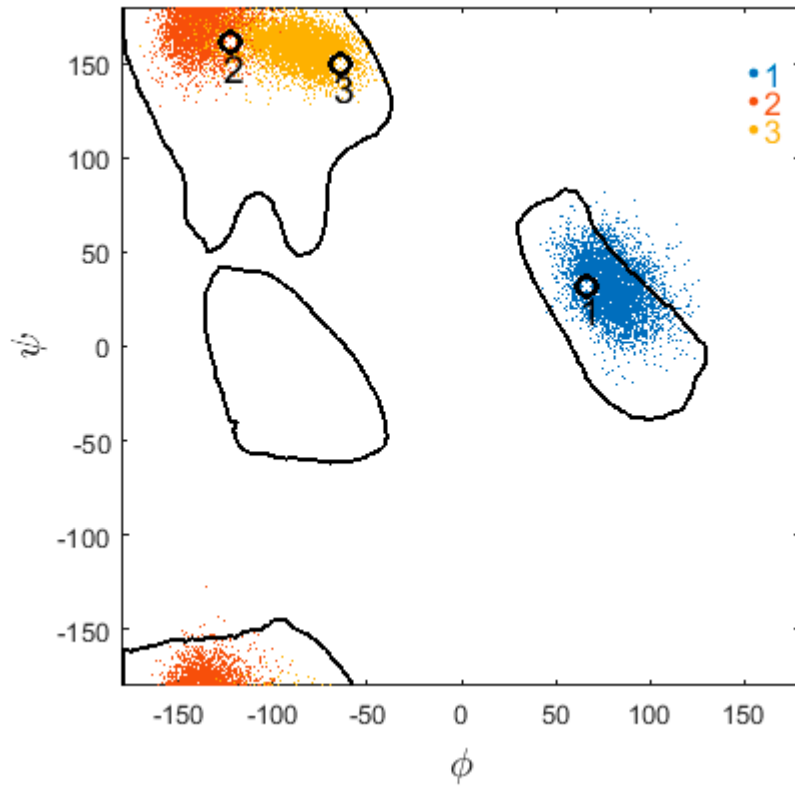
21 2AEK : 13 $\xi_p=100.0\%$ $S_p=100.0\%$



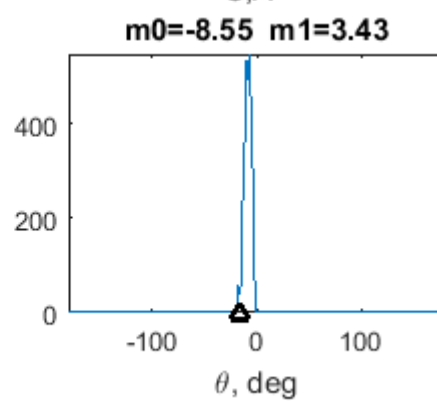
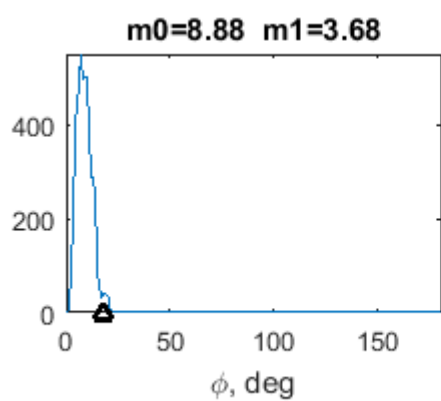
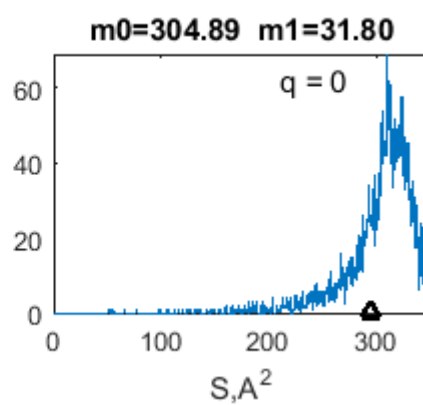
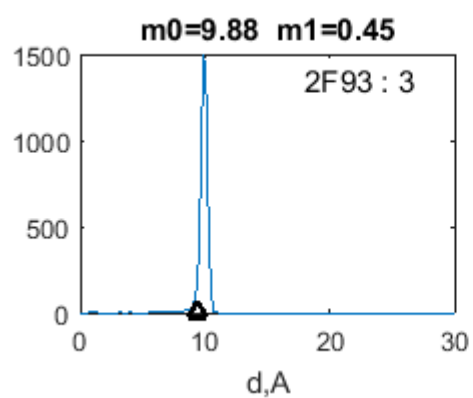
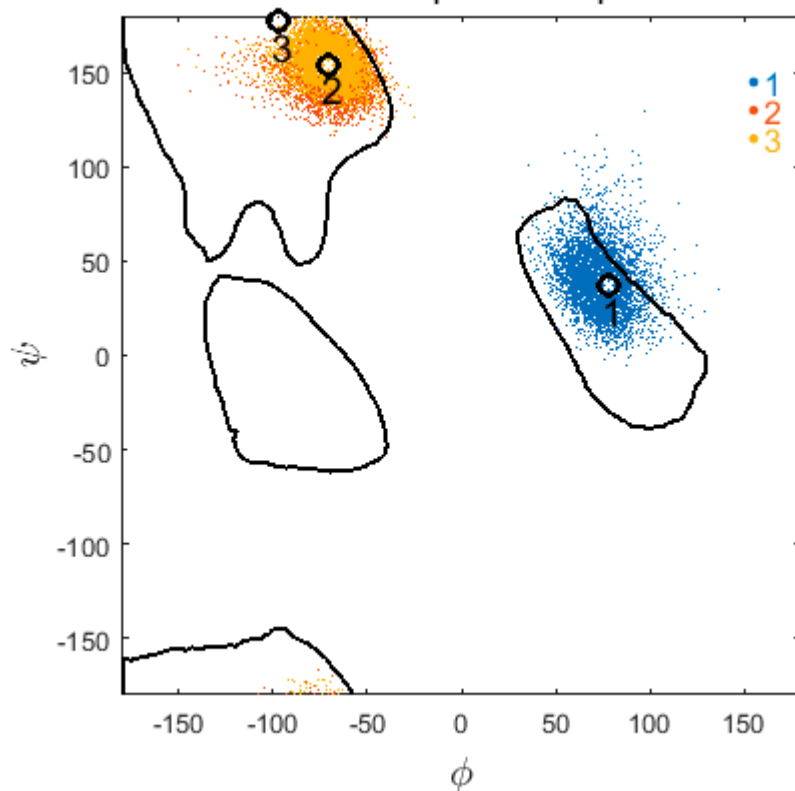
22 1PFU : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



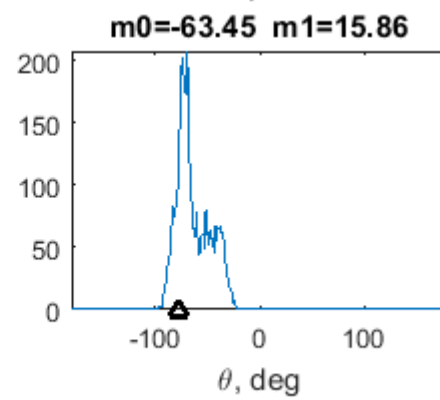
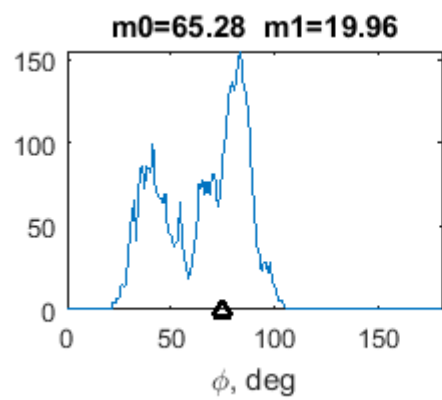
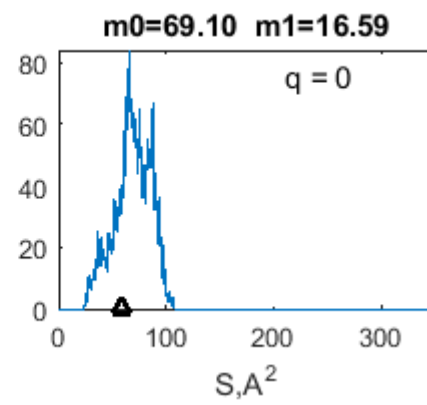
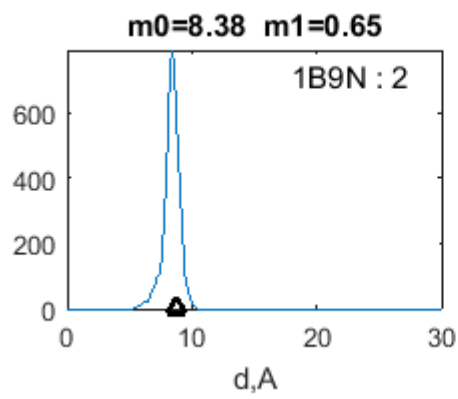
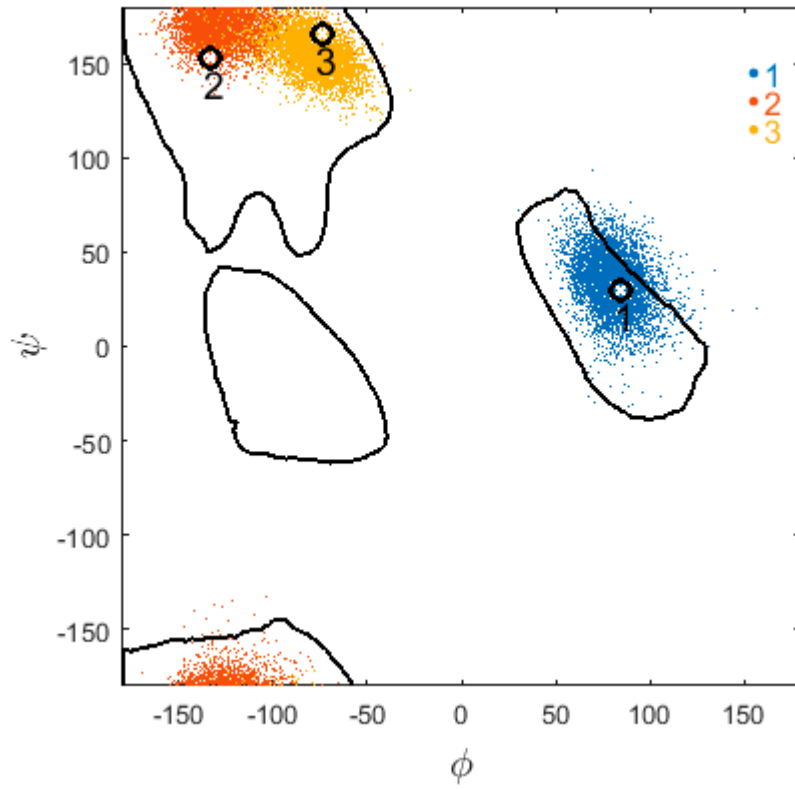
23 2OER : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



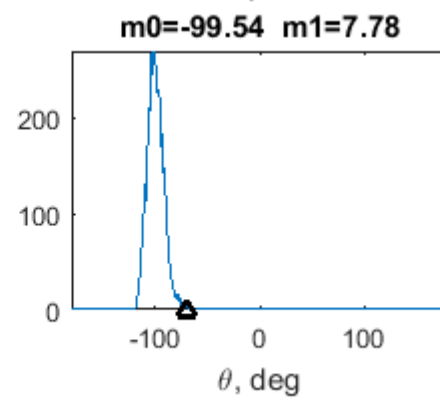
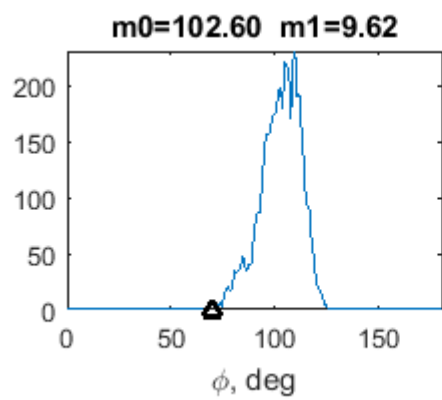
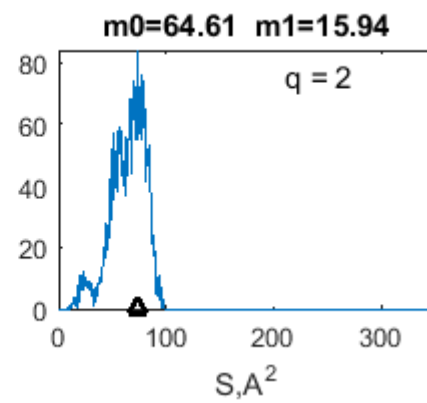
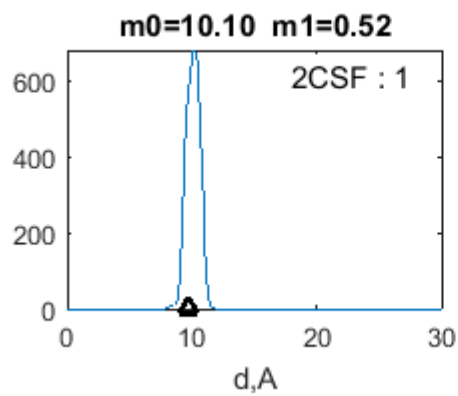
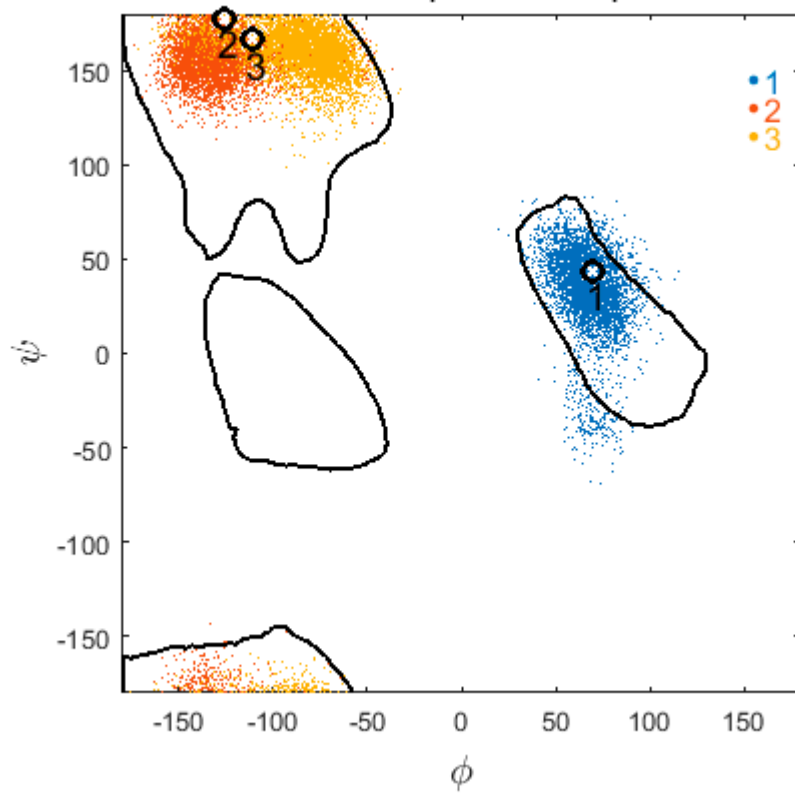
24 2F93 : 3 $\xi_p=99.9\%$ $S_p=100.0\%$



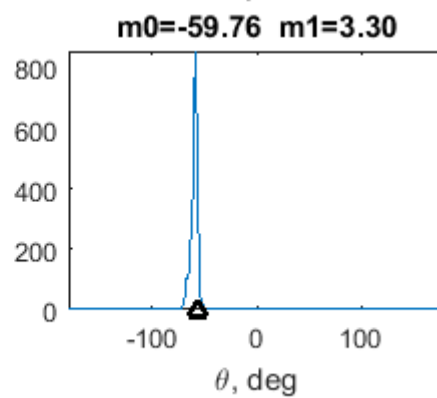
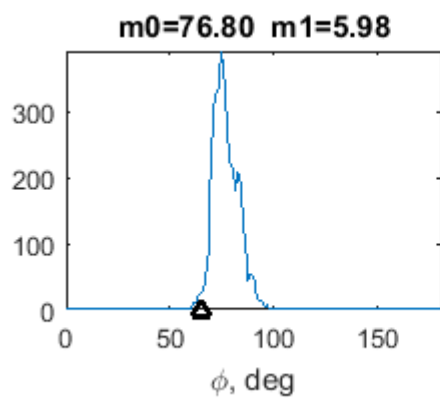
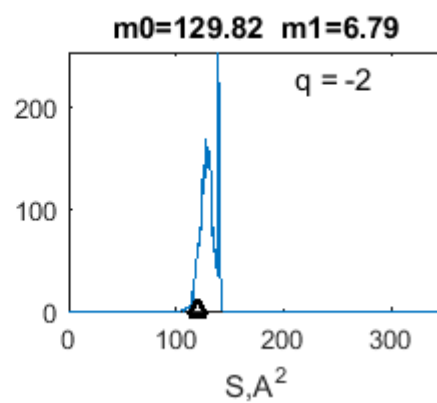
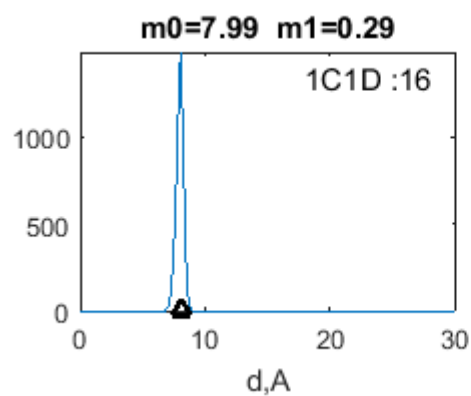
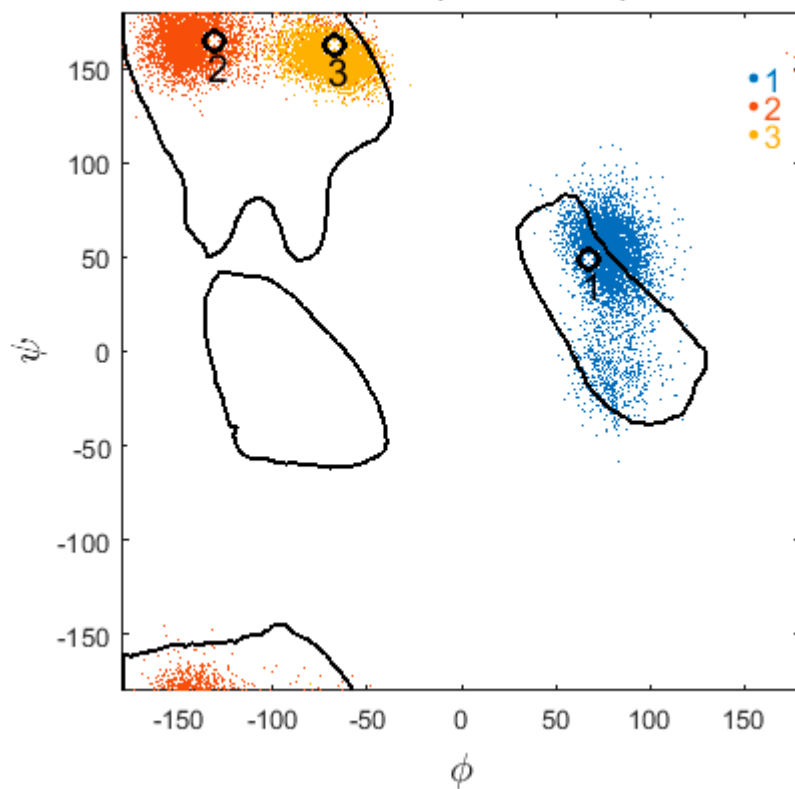
25 1B9N : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



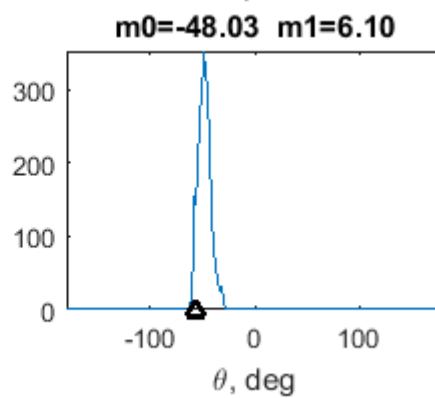
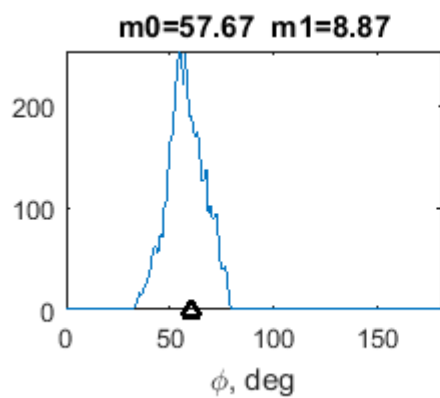
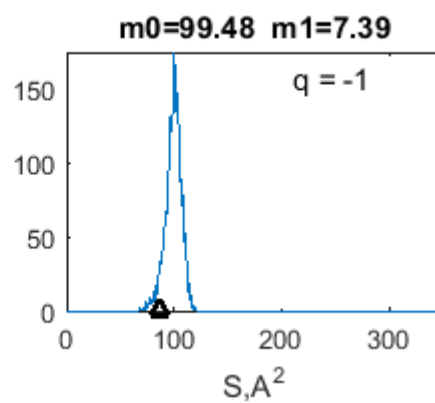
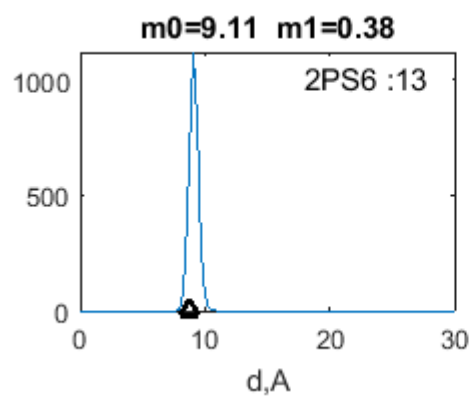
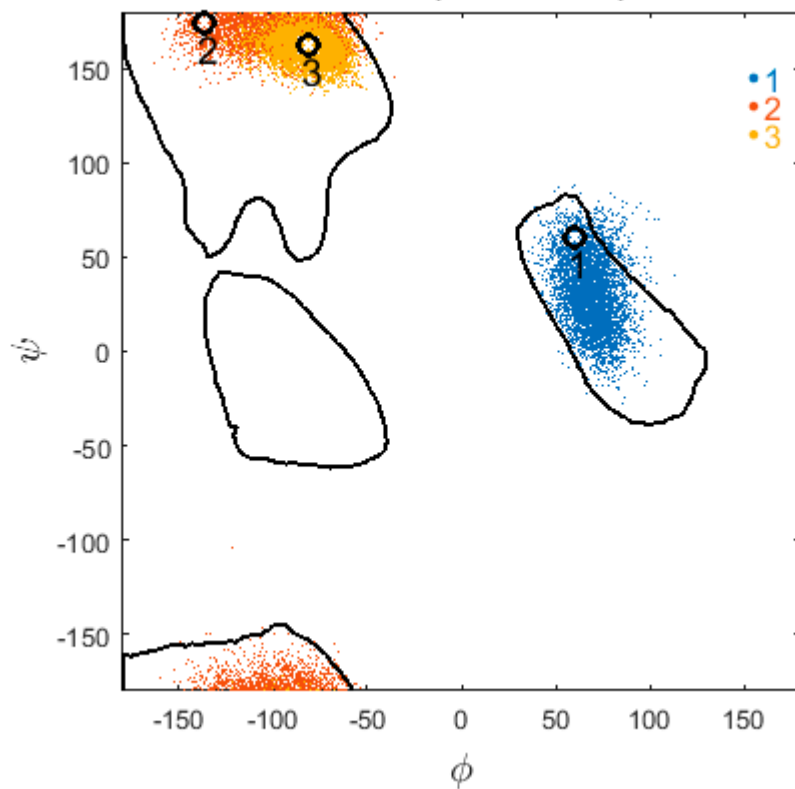
26 2CSF : 1 $\xi_p=100.0\%$ $S_p=100.0\%$



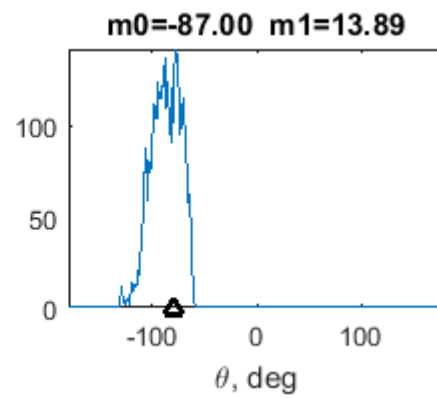
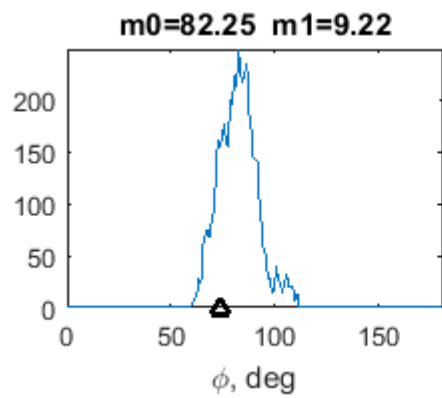
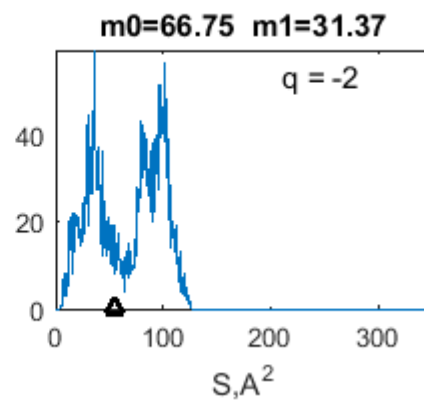
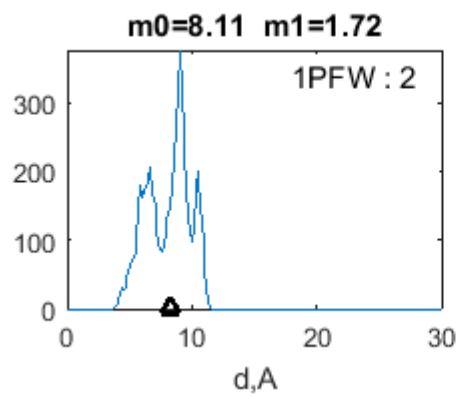
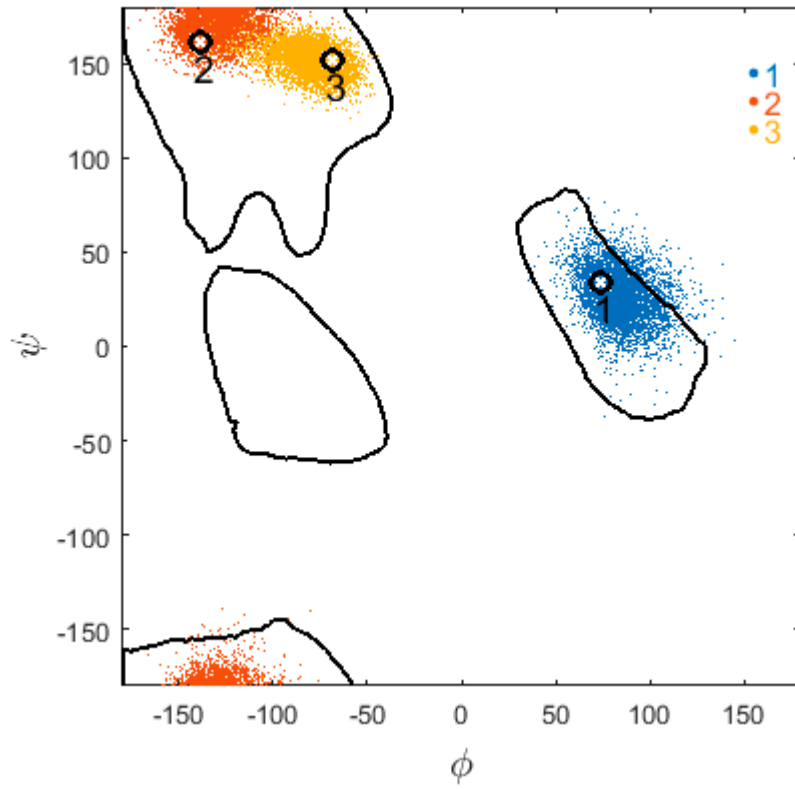
27 1C1D : 16 $\xi_p=100.0\%$ $S_p=100.0\%$



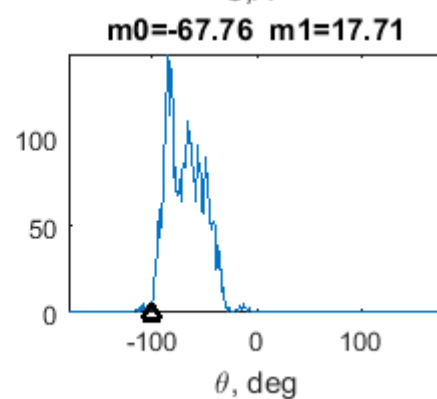
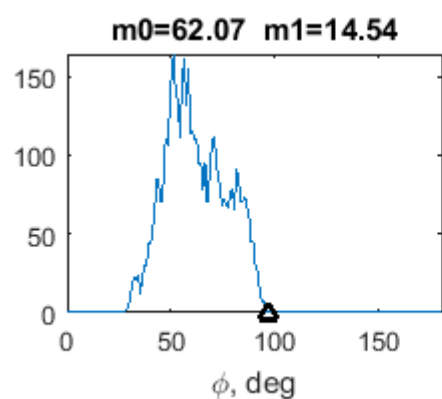
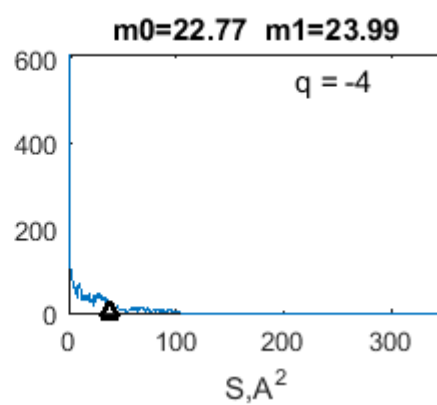
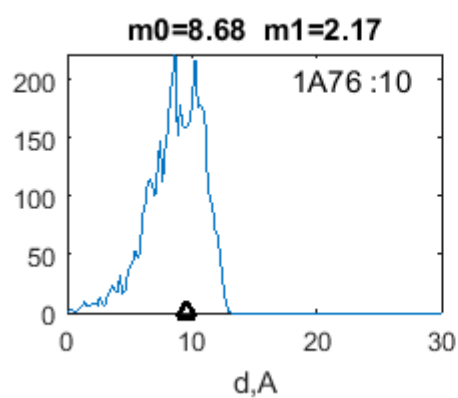
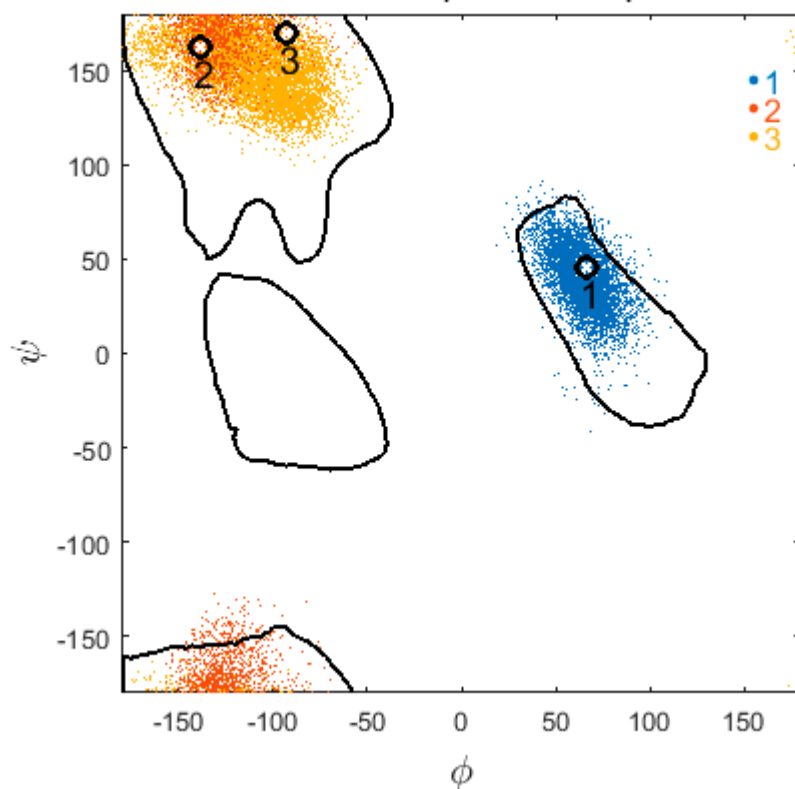
28 2PS6 : 13 $\xi_p=100.0\%$ $S_p=100.0\%$



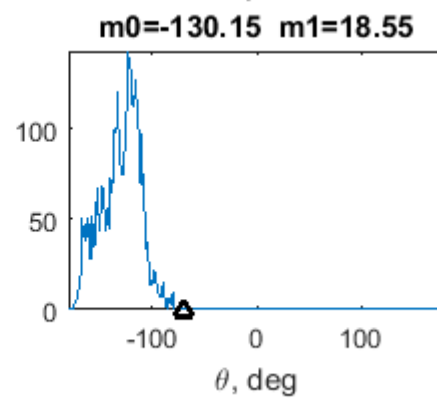
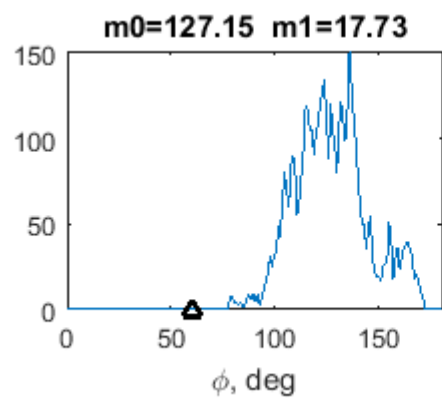
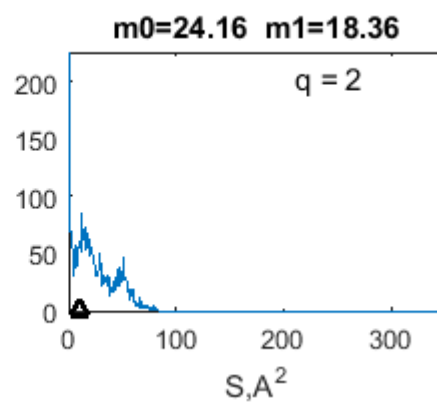
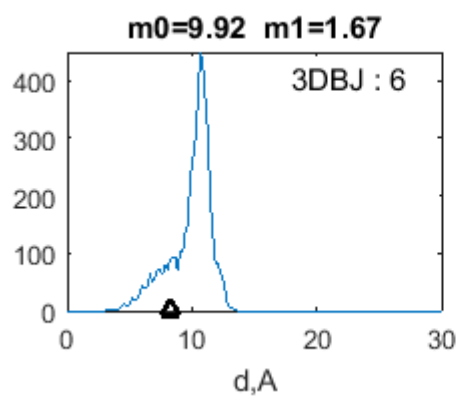
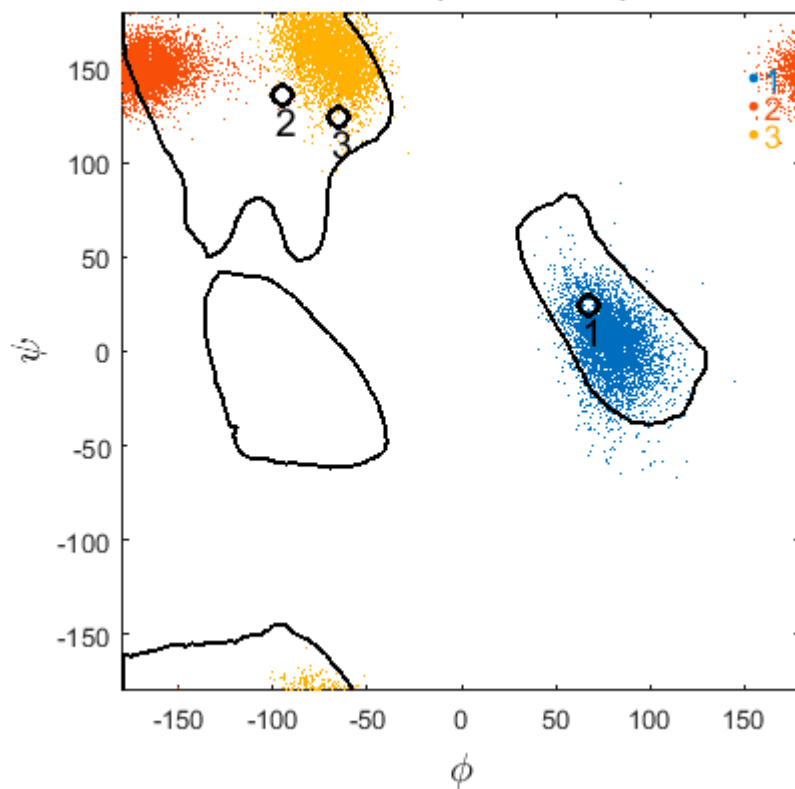
30 1PFW : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



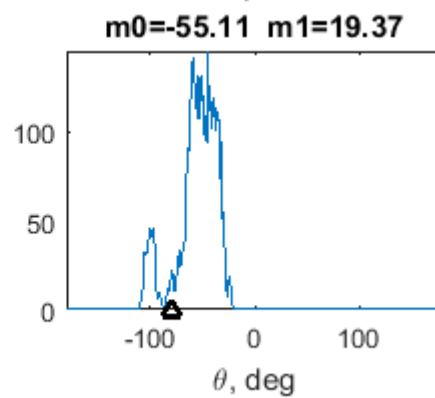
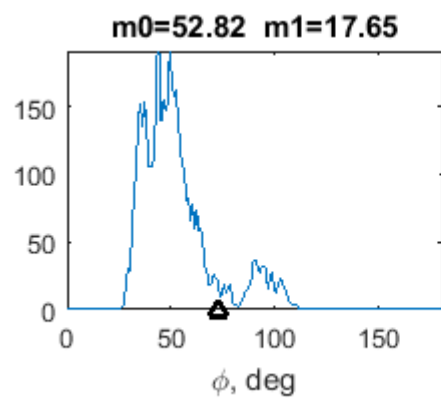
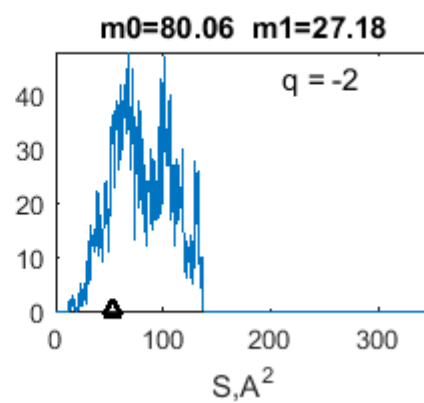
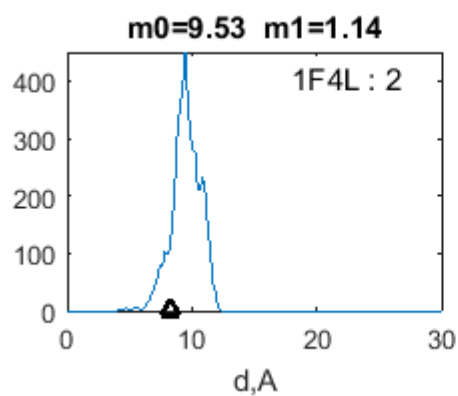
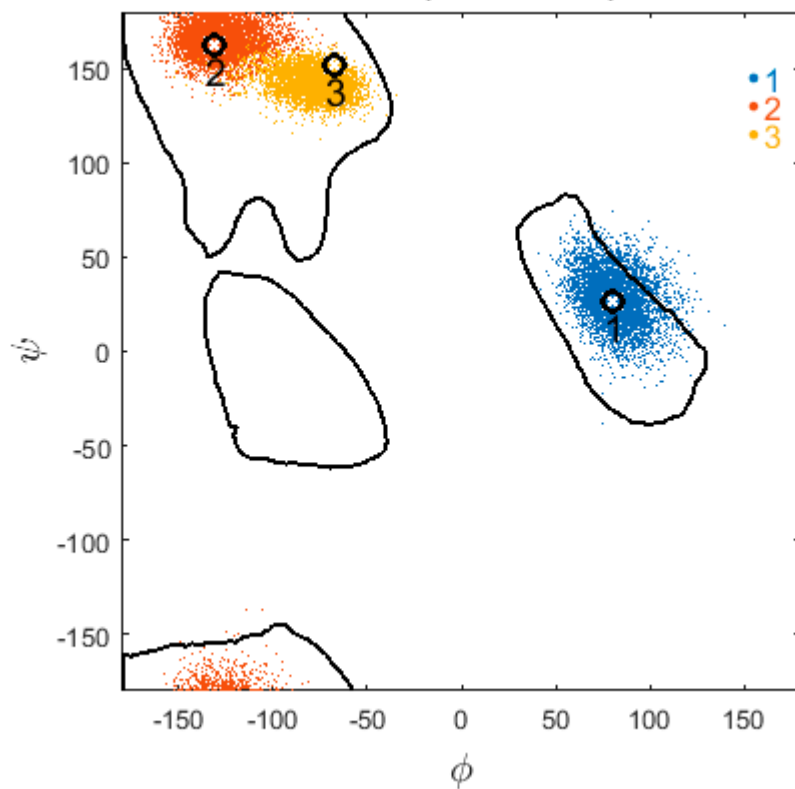
31 1A76 : 10 $\xi_p=100.0\%$ $S_p=92.0\%$



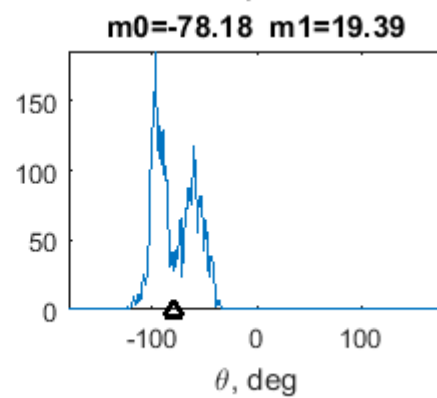
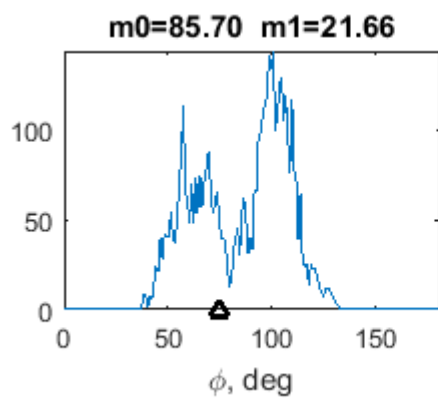
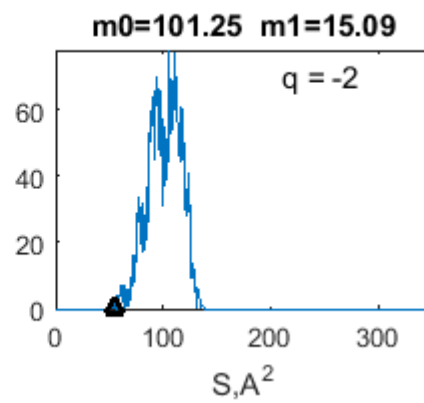
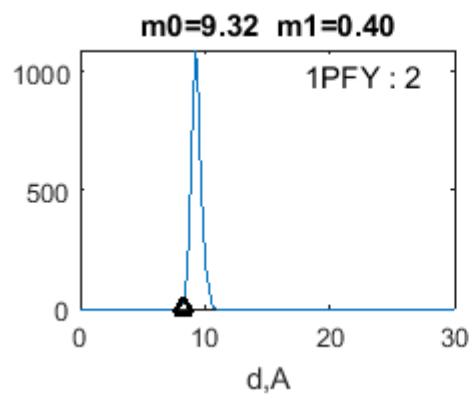
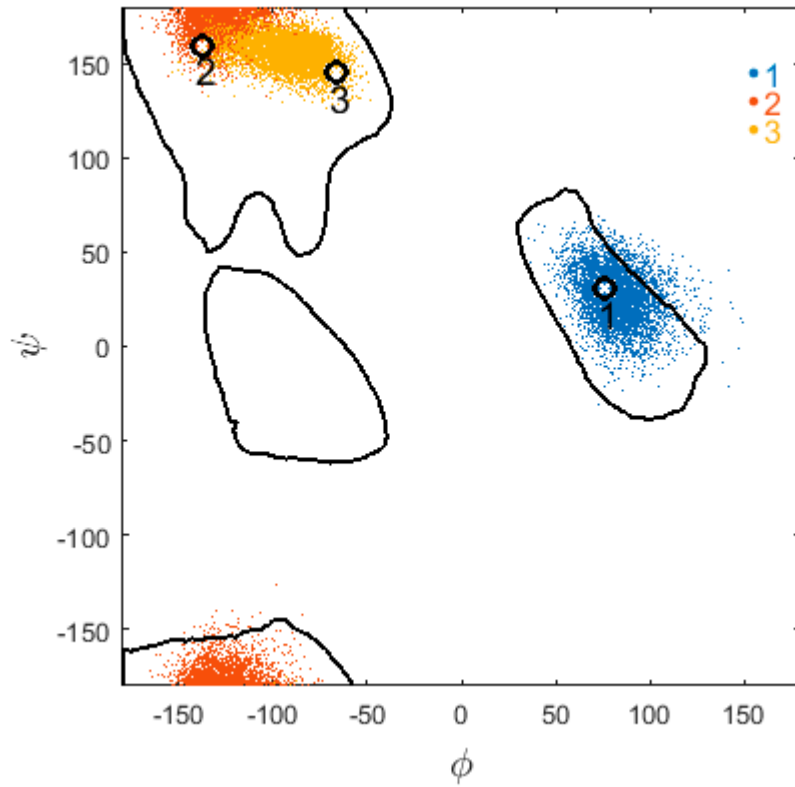
32 3DBJ : 6 $\xi_p=100.0\%$ $S_p=97.1\%$



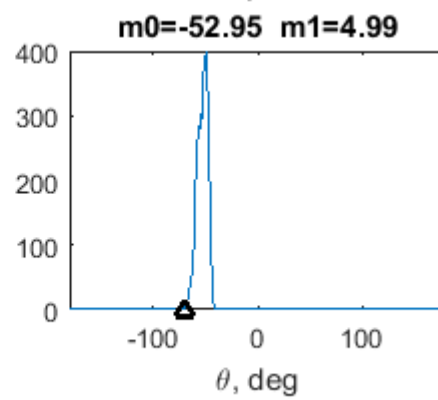
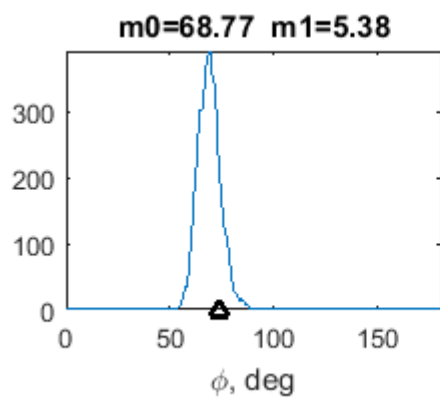
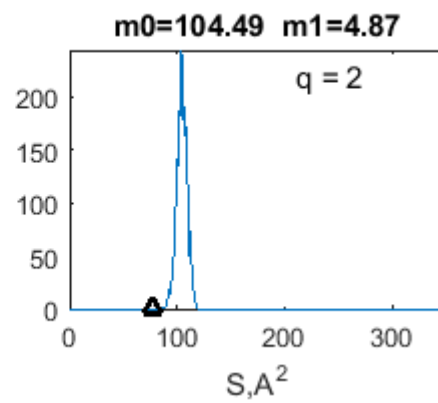
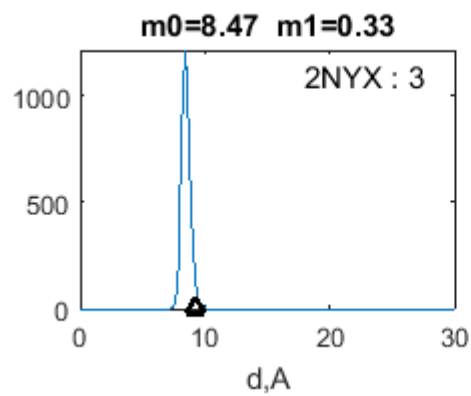
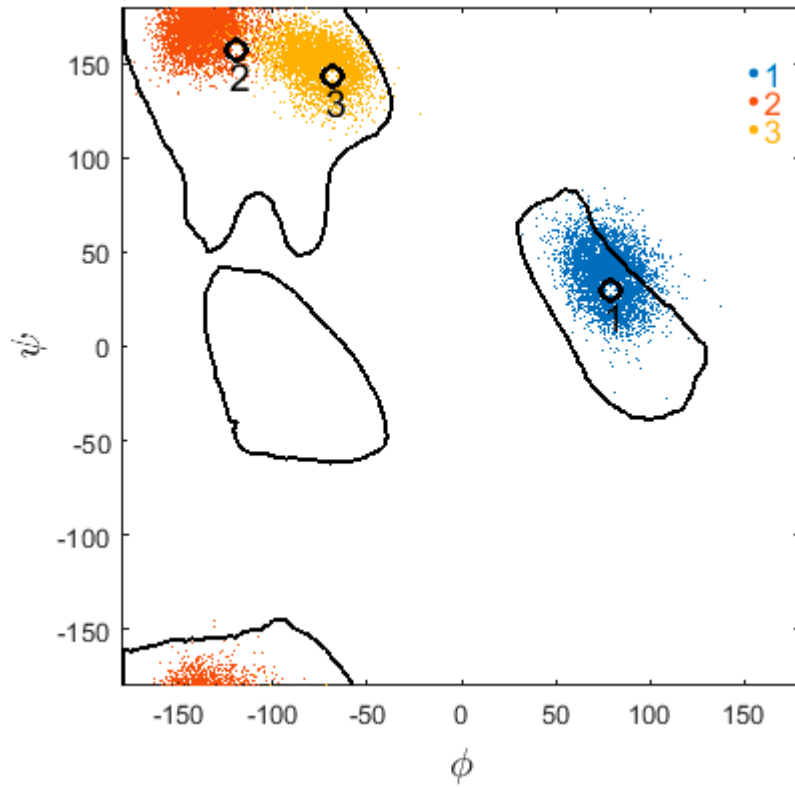
34 1F4L : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



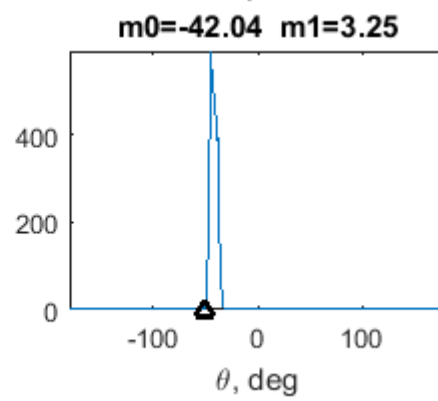
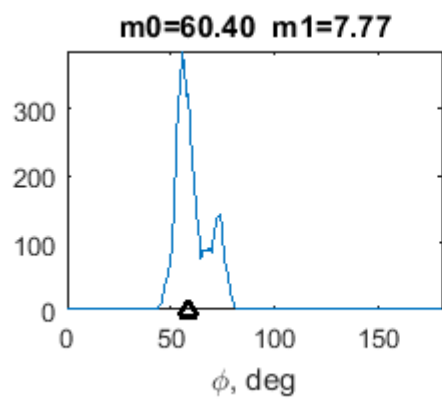
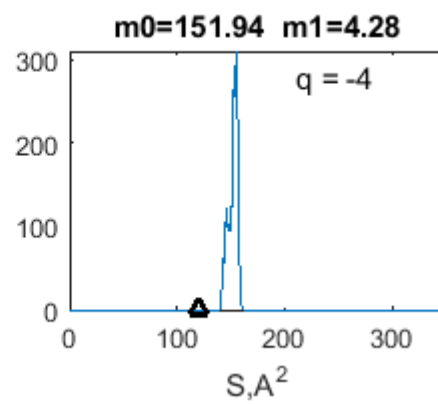
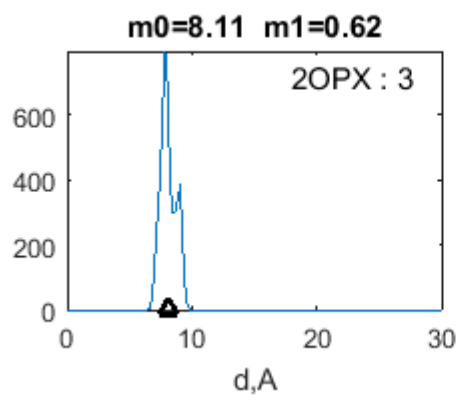
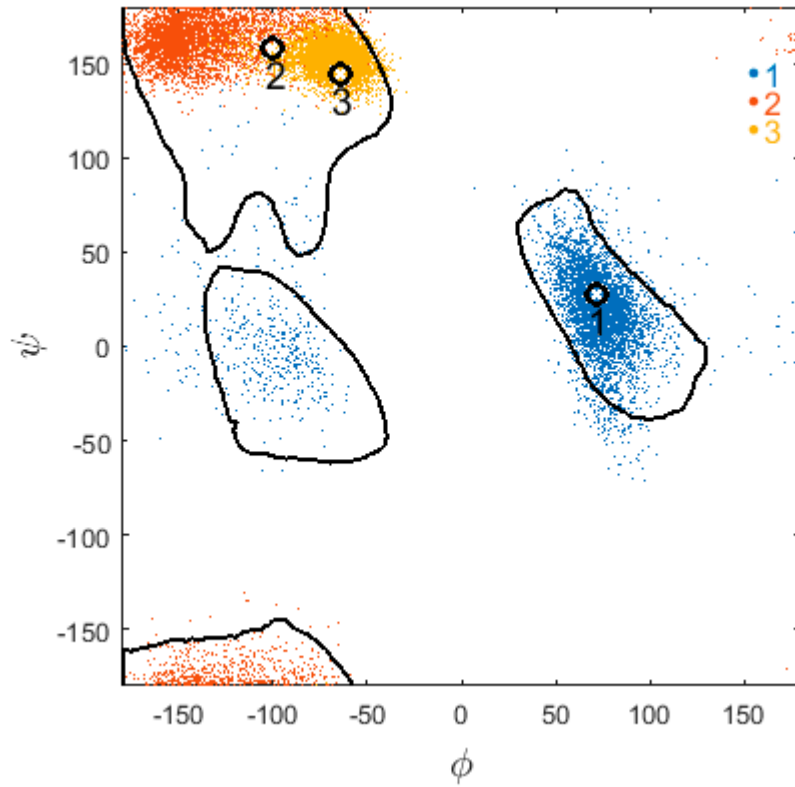
37 1PFY : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



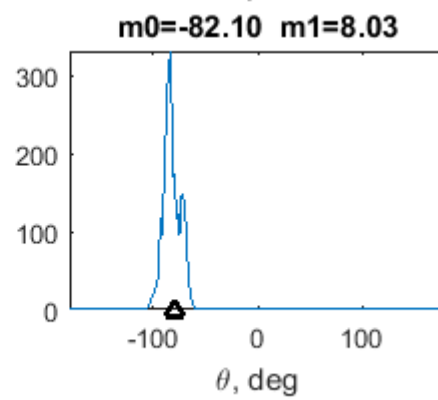
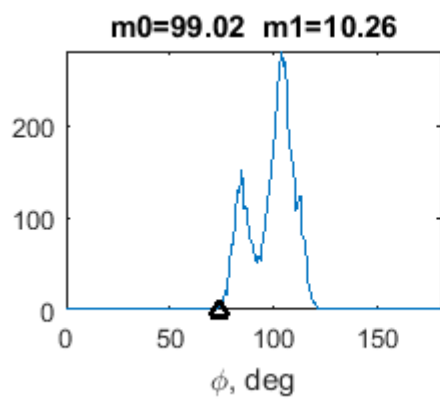
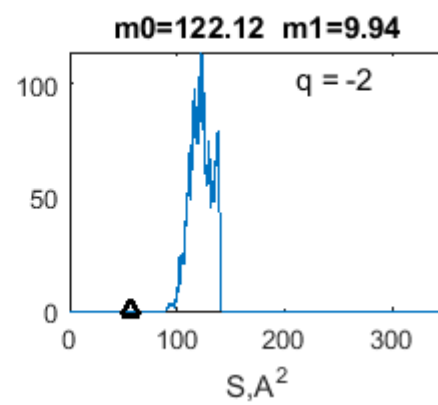
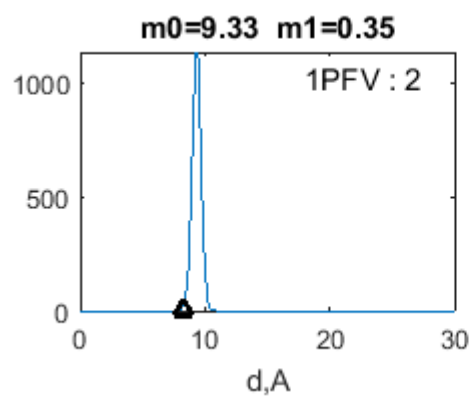
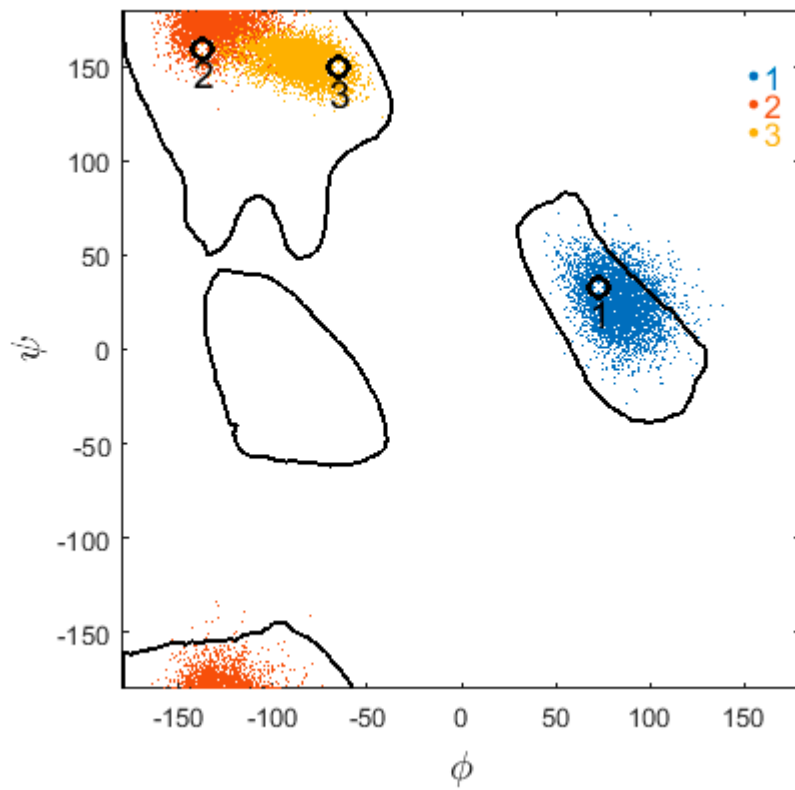
38 2NYX : 3 $\xi_p=100.0\%$ $S_p=100.0\%$



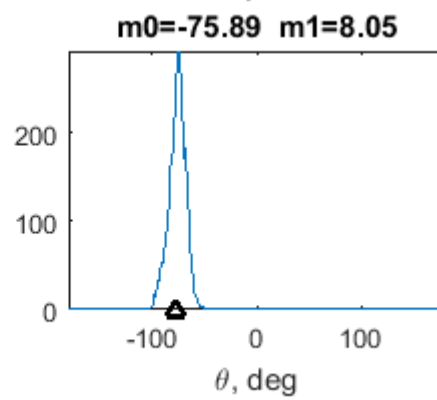
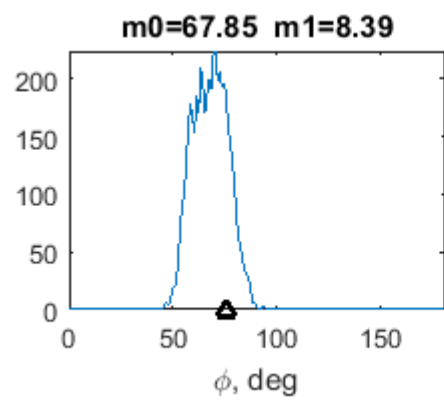
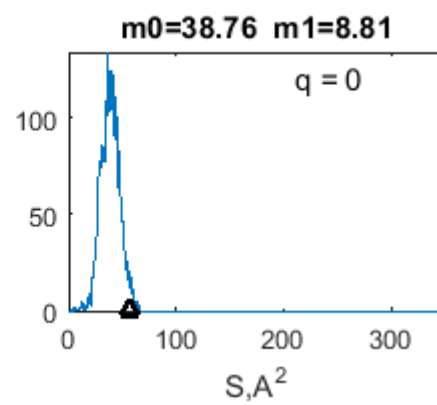
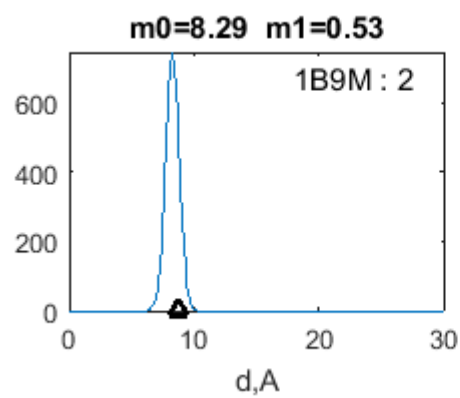
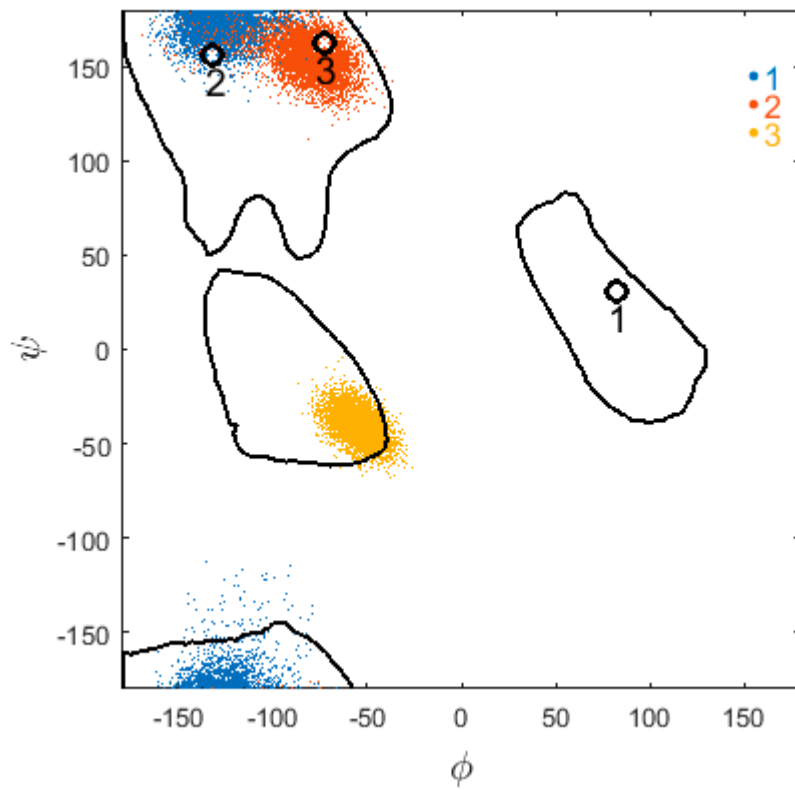
39 2OPX : 3 $\xi_p=100.0\%$ $S_p=100.0\%$



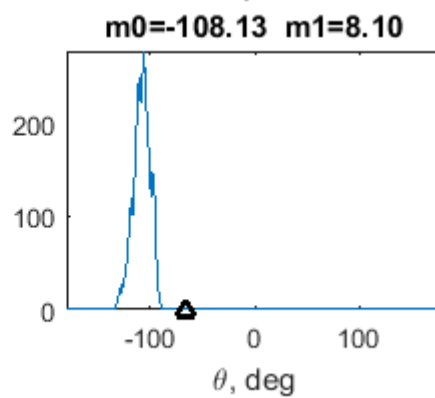
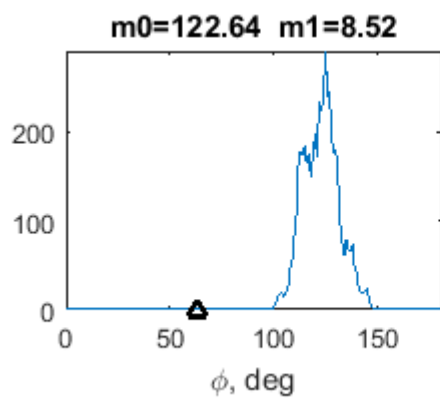
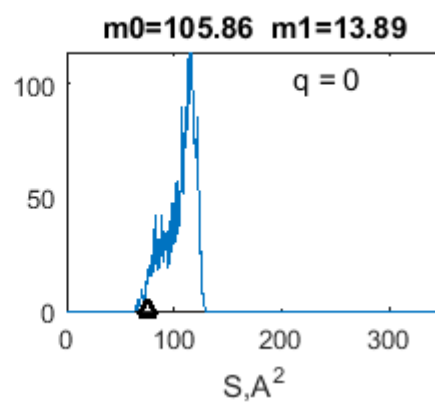
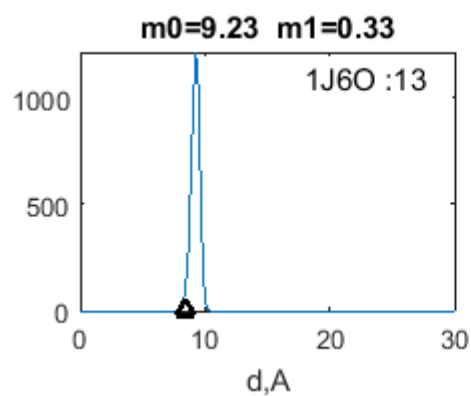
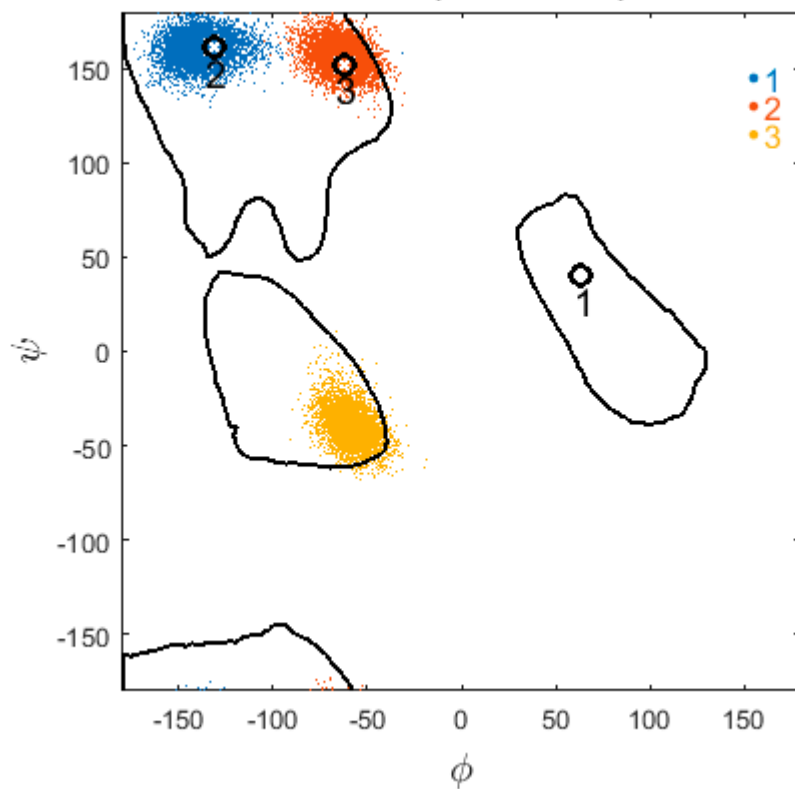
41 1PFV : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



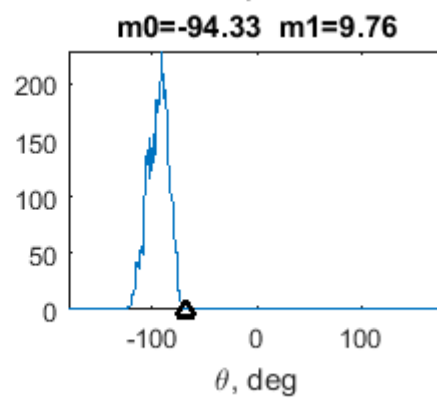
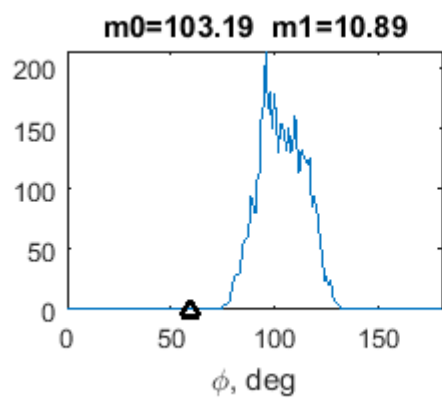
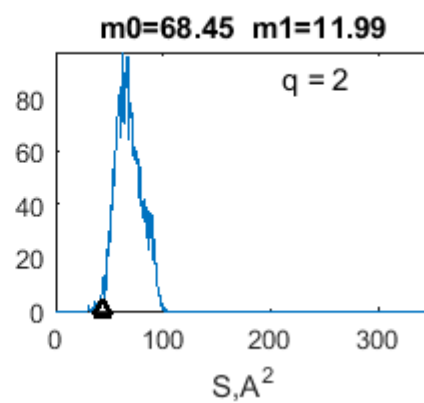
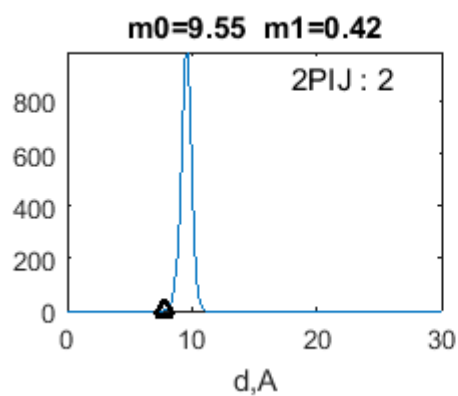
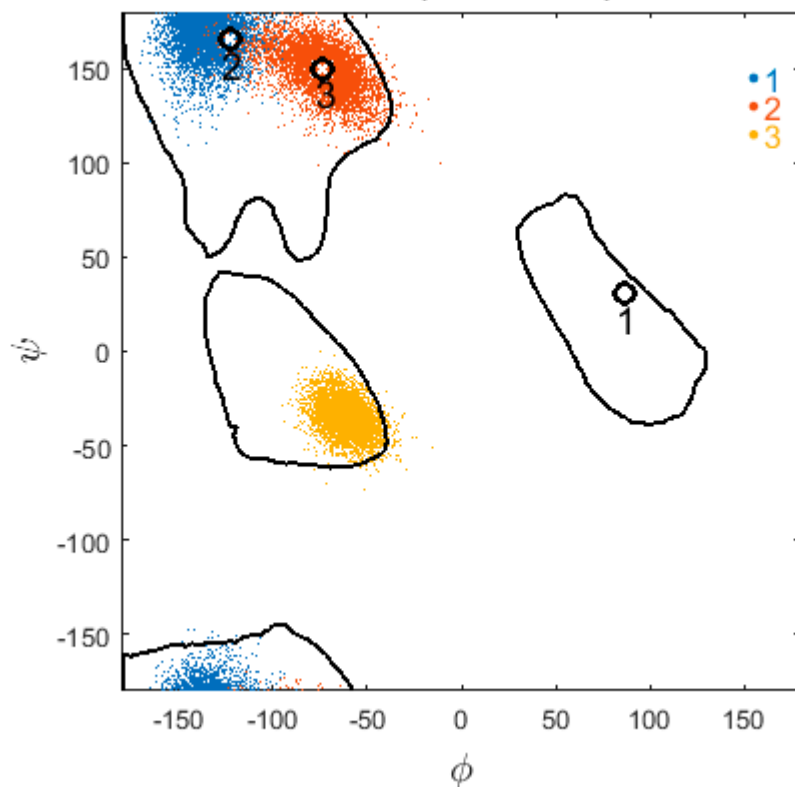
10 1B9M : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



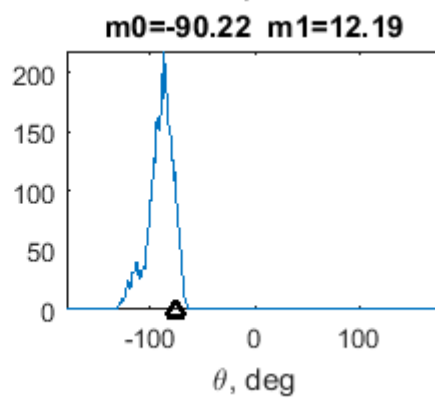
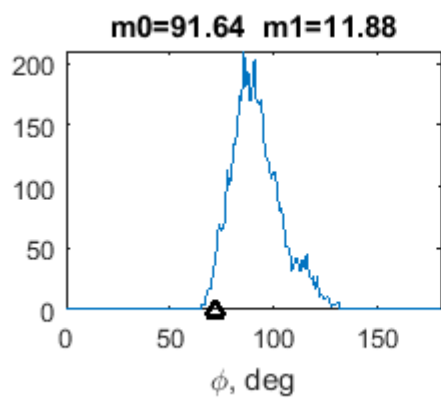
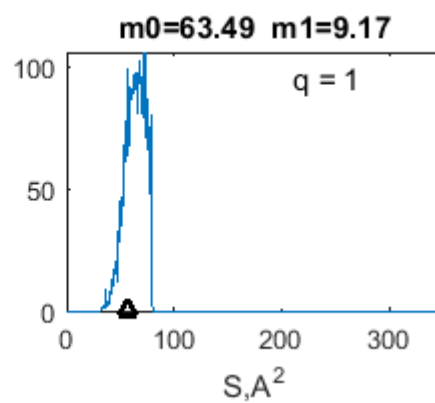
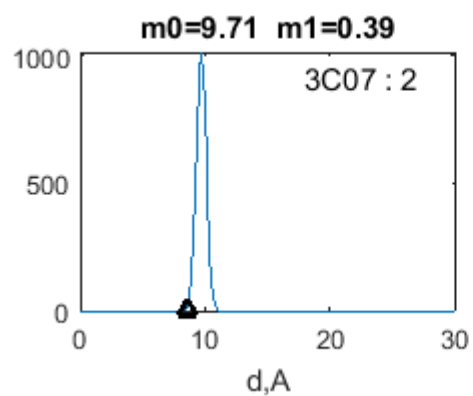
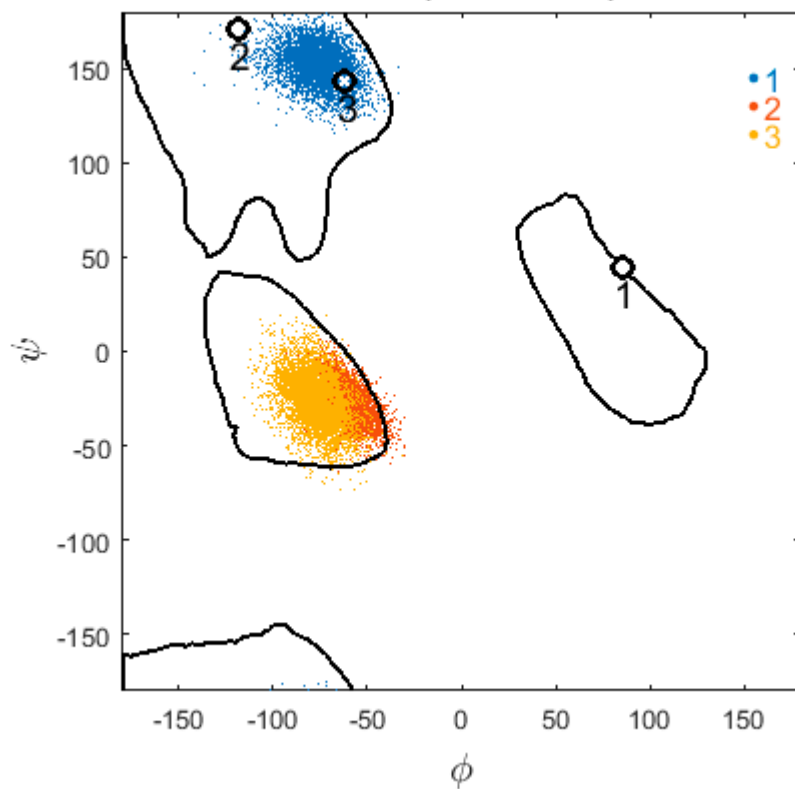
29 1J6O : 13 $\xi_p=100.0\%$ $S_p=100.0\%$



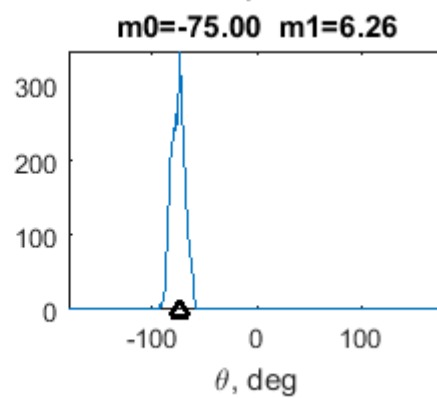
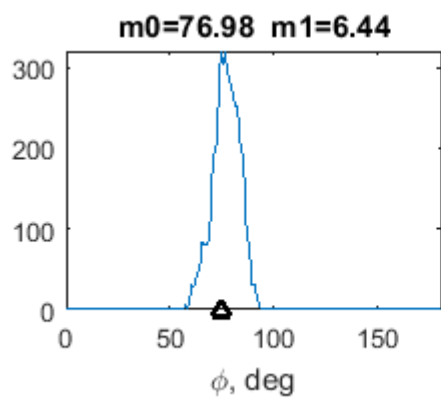
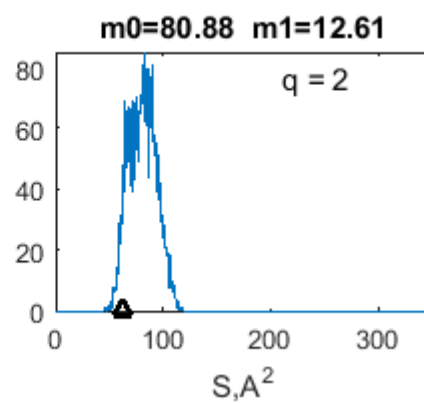
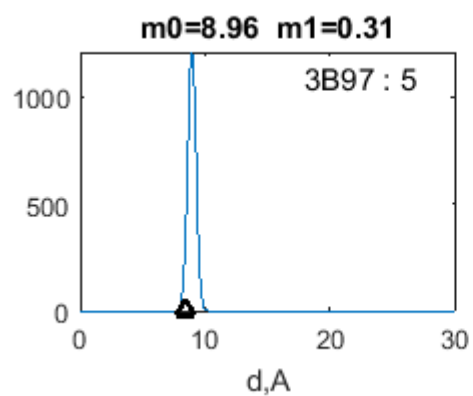
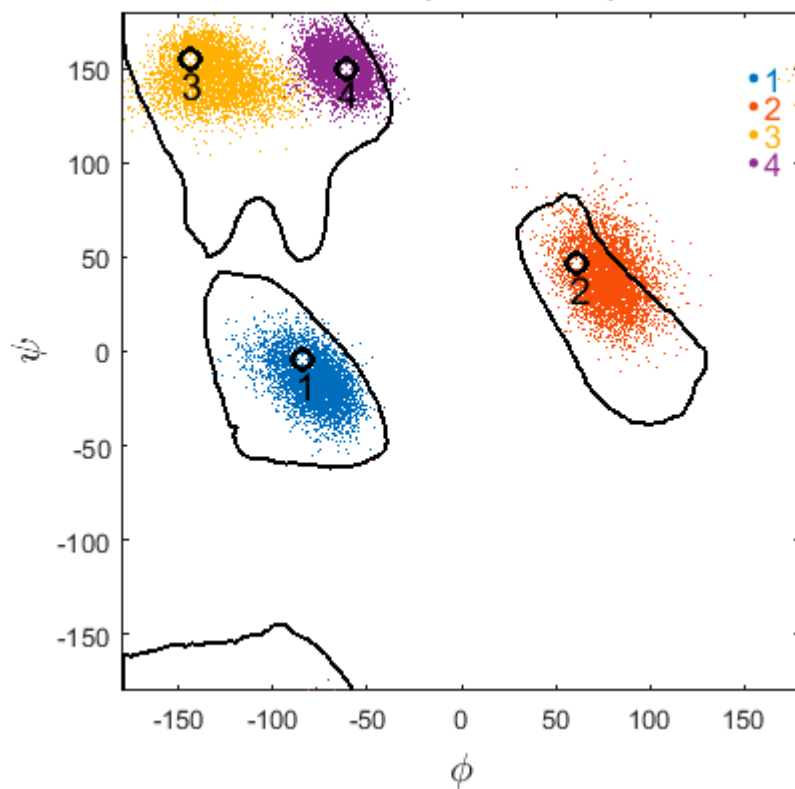
40 2PIJ : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



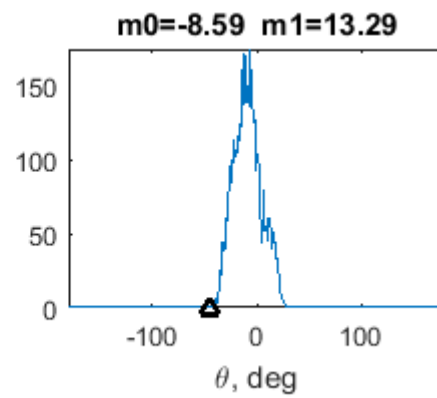
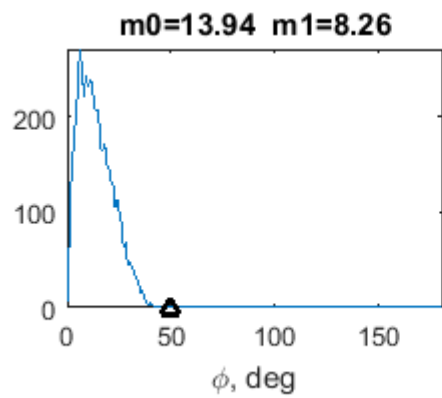
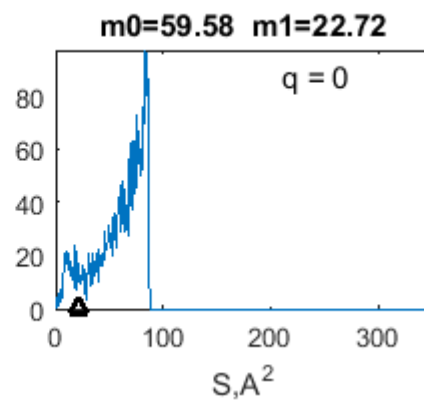
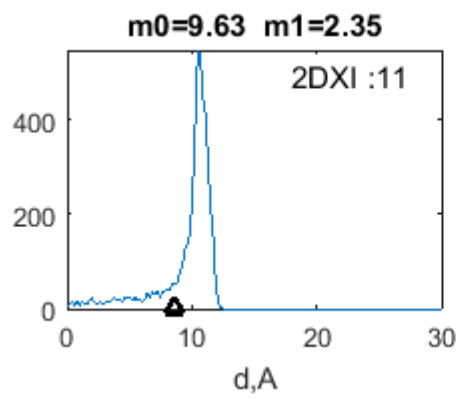
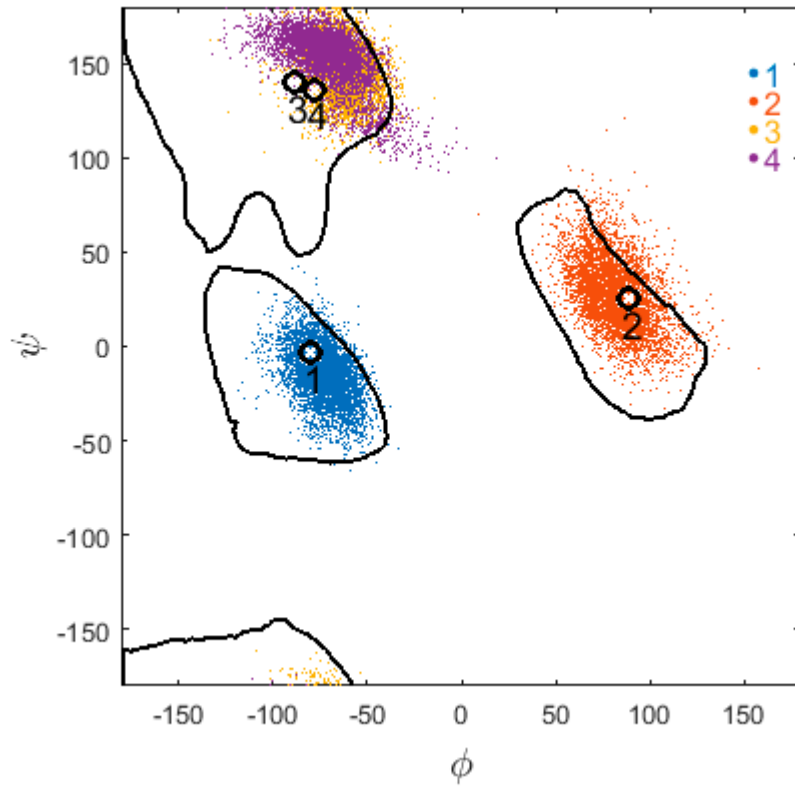
11 3C07 : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



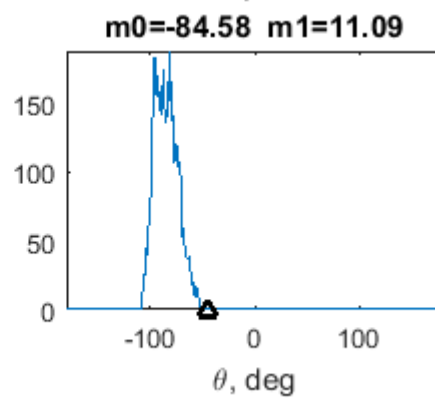
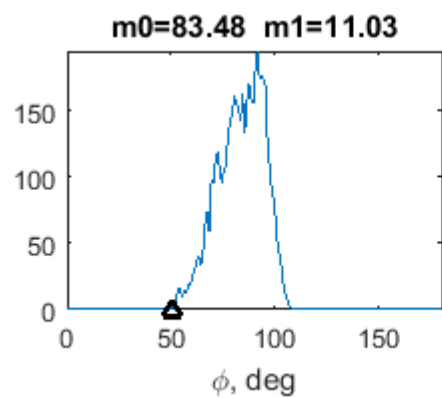
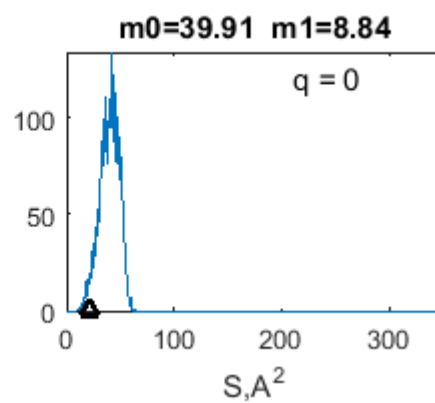
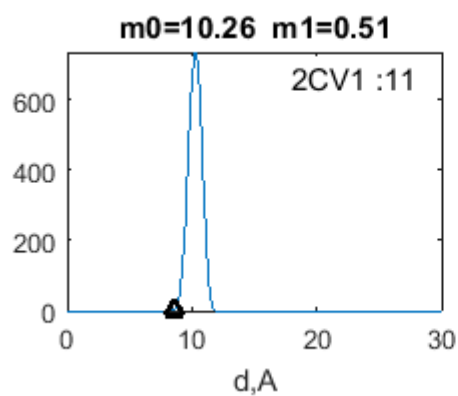
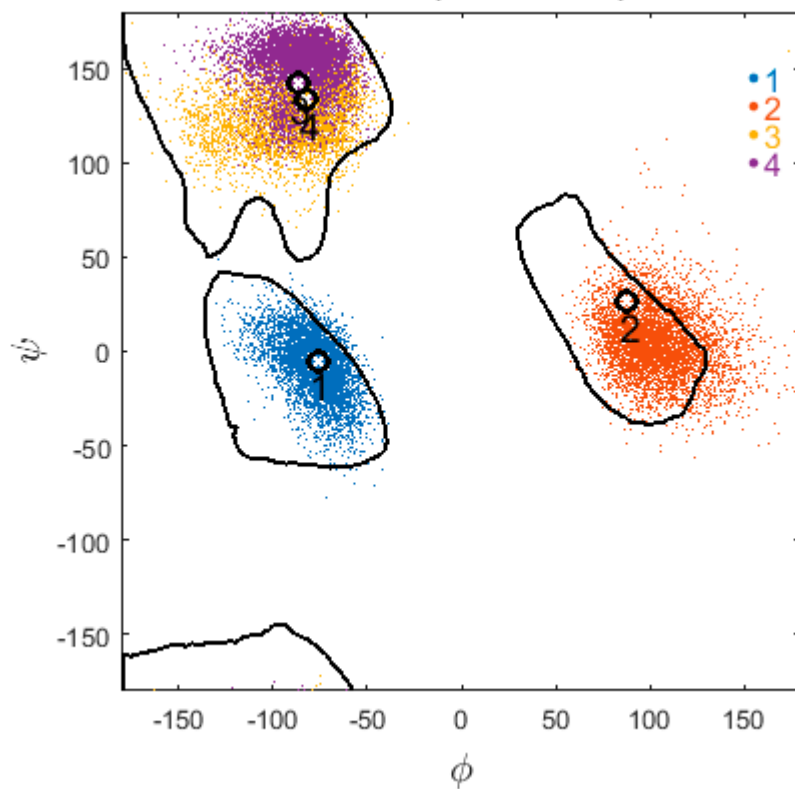
42 3B97 : 5 $\xi_p=100.0\%$ $S_p=100.0\%$



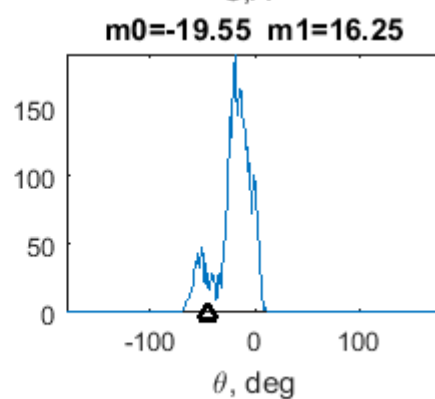
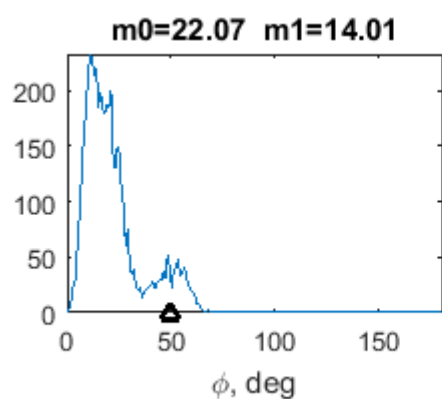
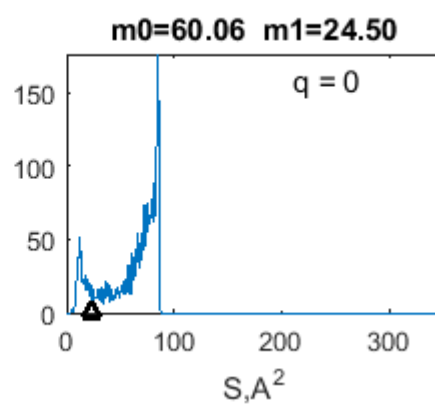
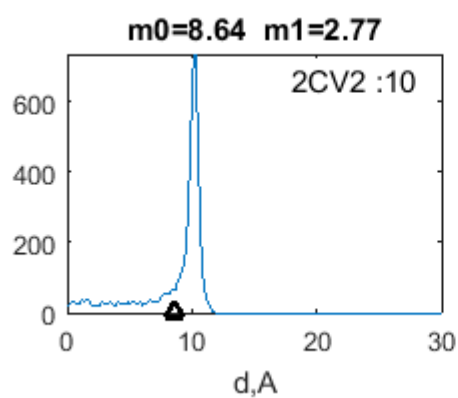
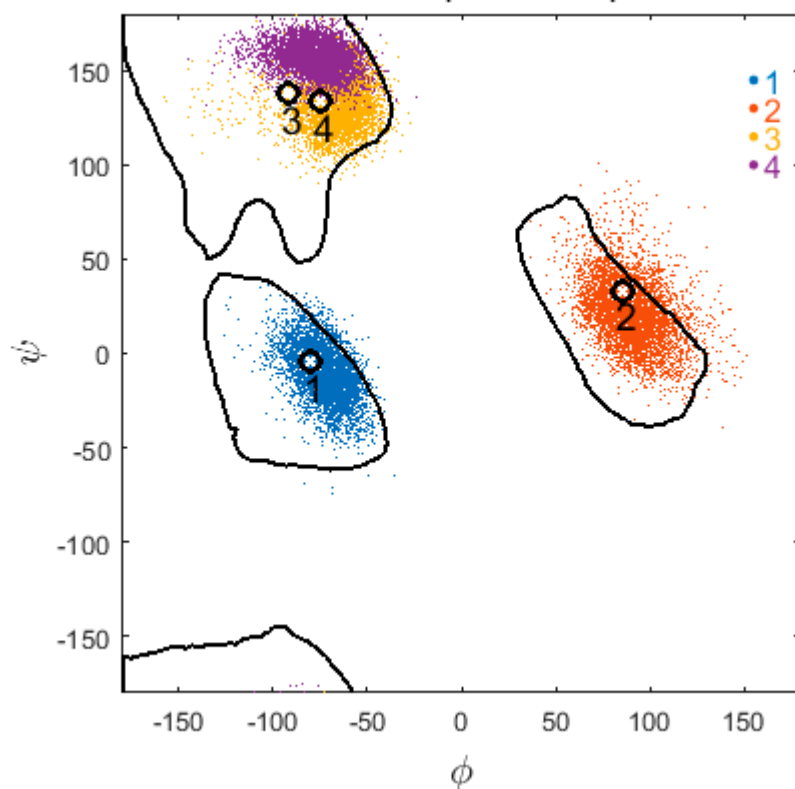
44 2DXI : 11 $\xi_p=75.3\%$ $S_p=100.0\%$



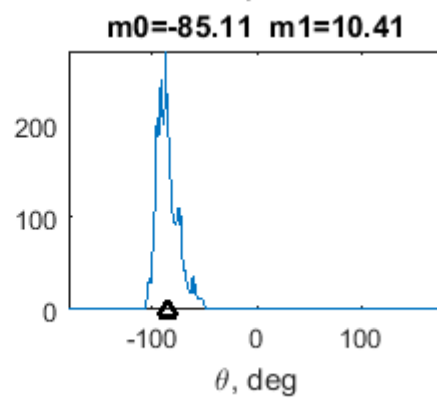
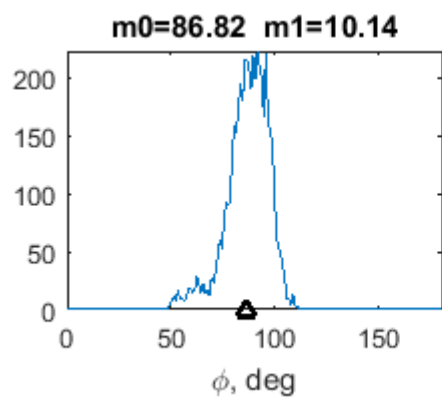
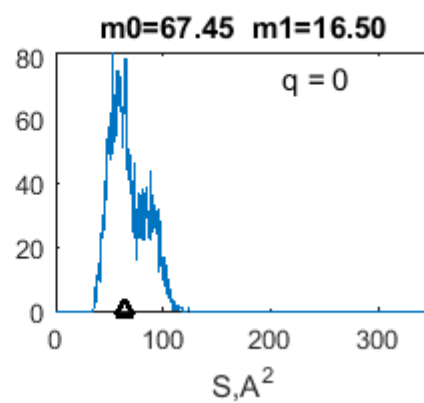
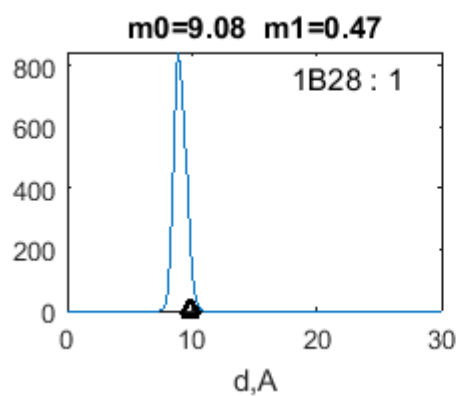
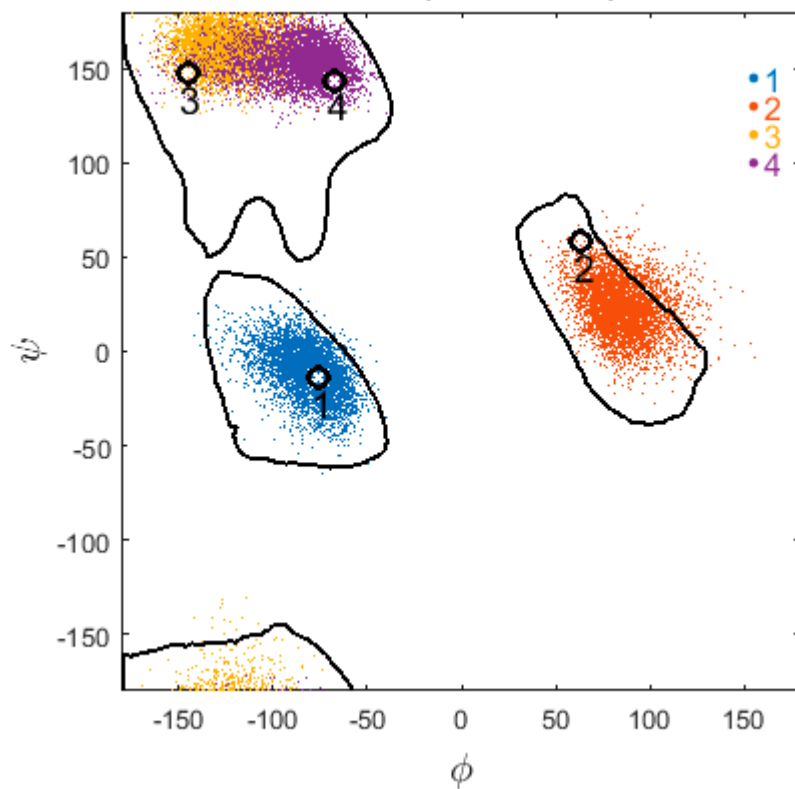
46 2CV1 : 11 $\xi_p=100.0\%$ $S_p=100.0\%$



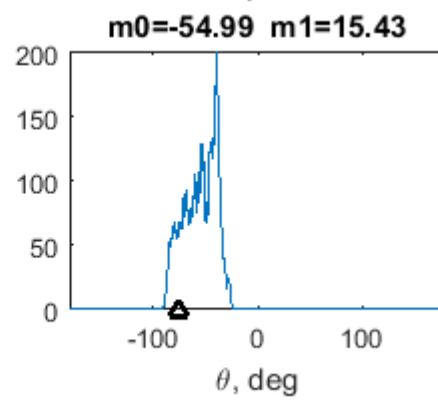
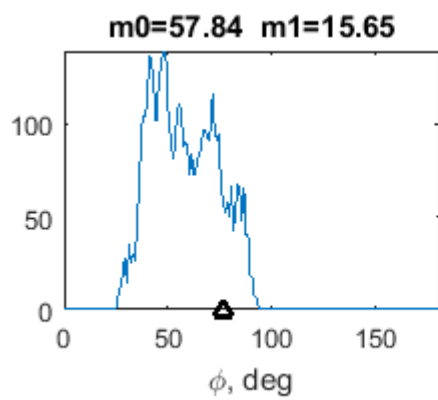
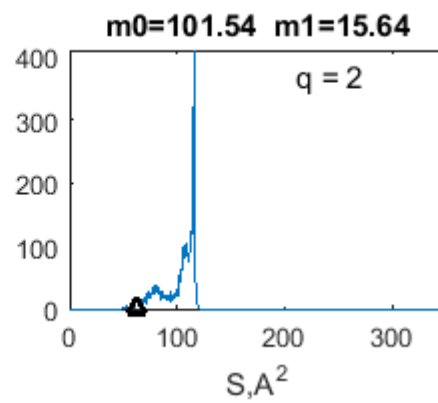
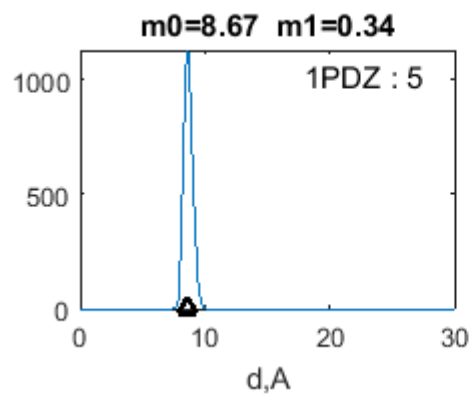
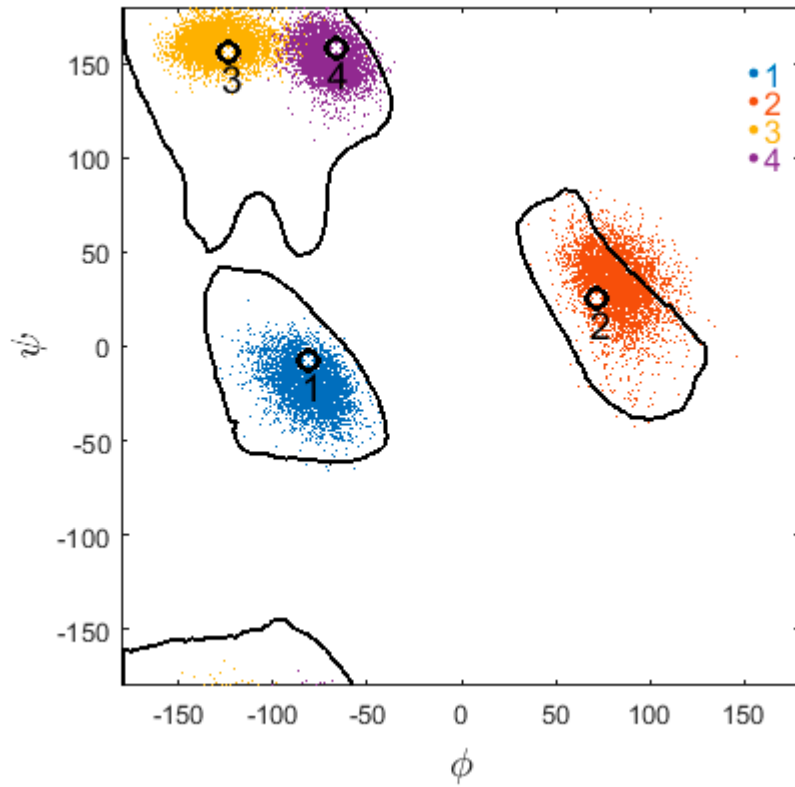
47 2CV2 : 10 $\xi_p=91.7\%$ $S_p=100.0\%$



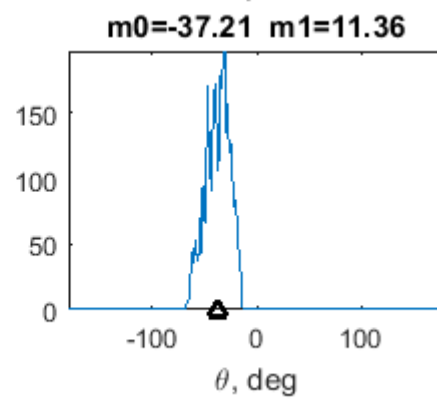
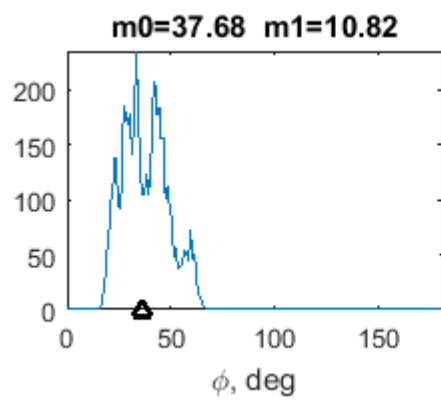
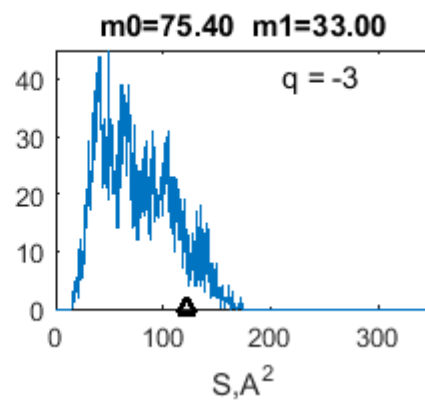
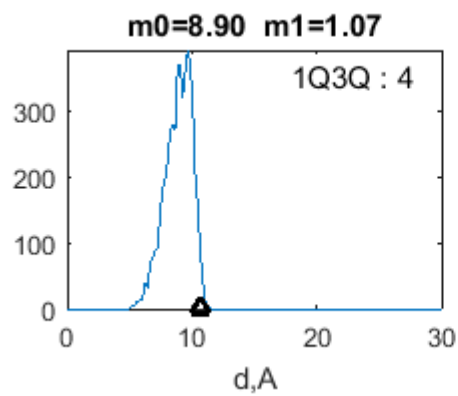
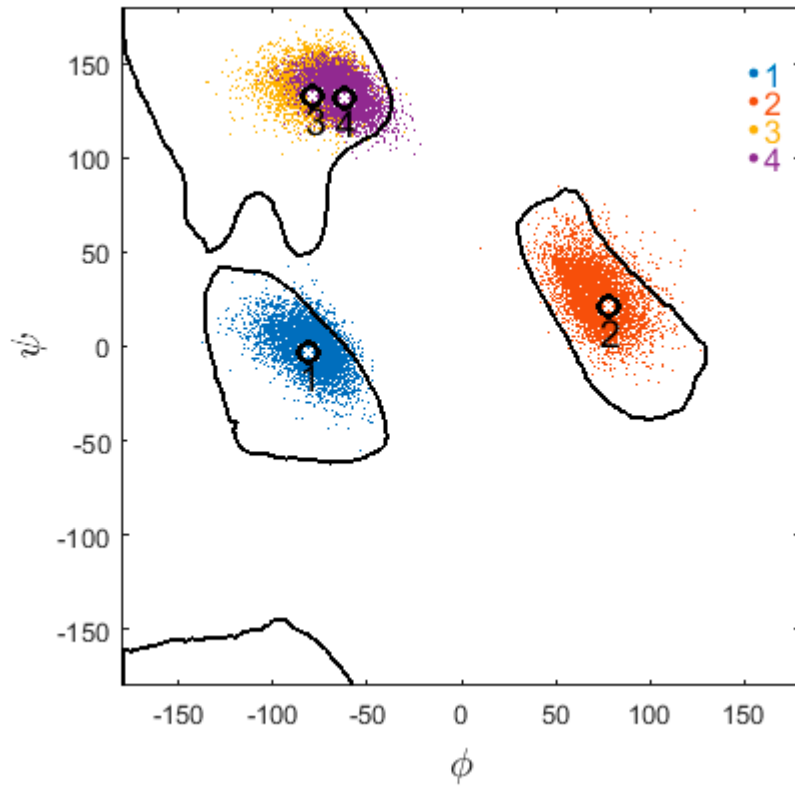
48 1B28 : 1 $\xi_p=100.0\%$ $S_p=100.0\%$



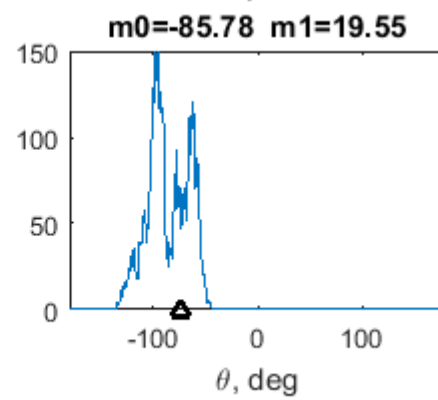
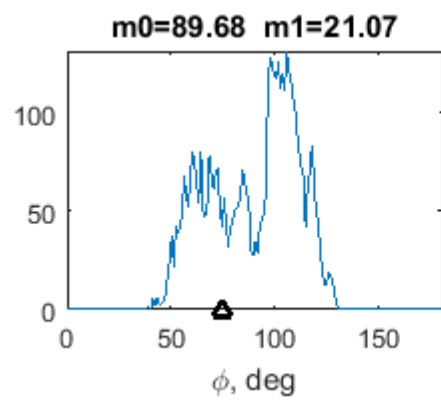
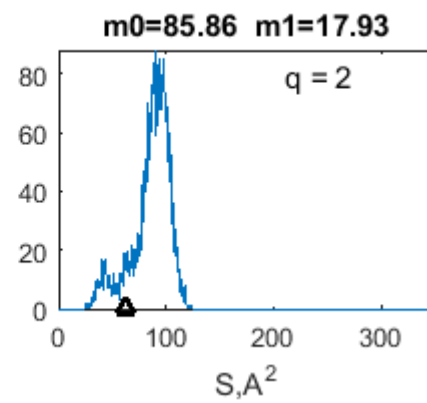
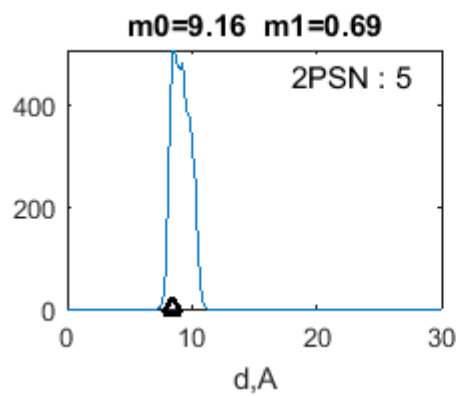
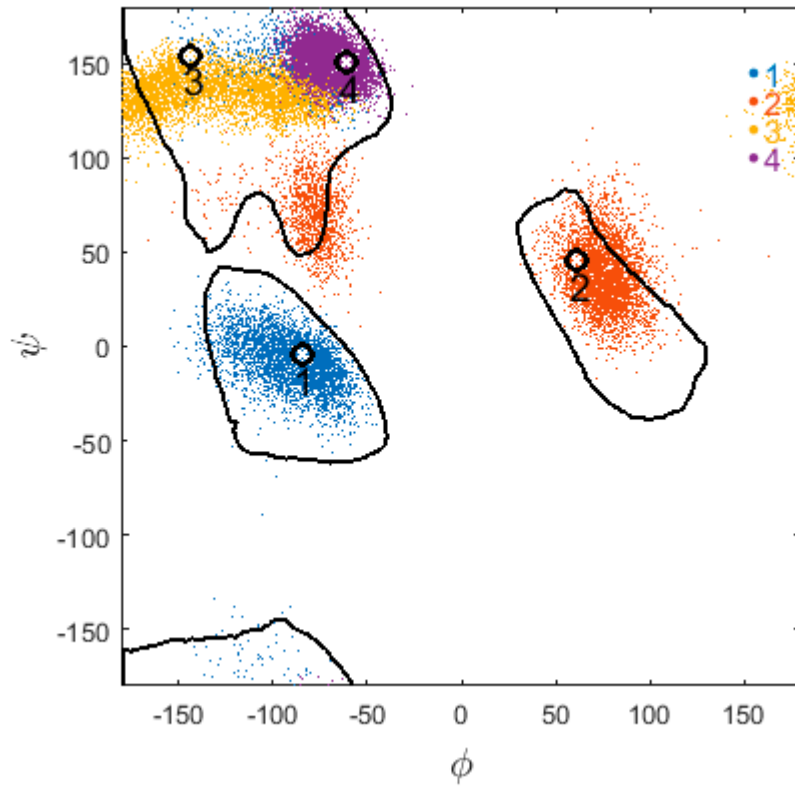
50 1PDZ : 5 $\xi_p=100.0\%$ $S_p=100.0\%$



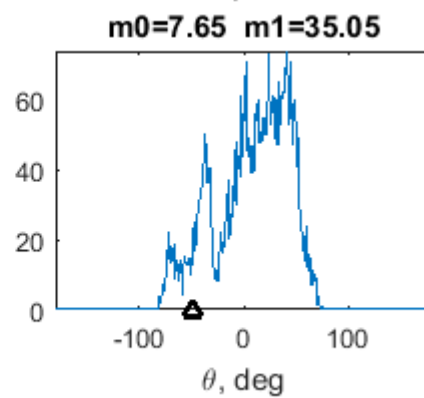
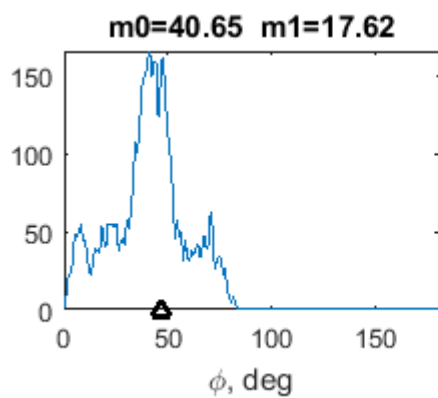
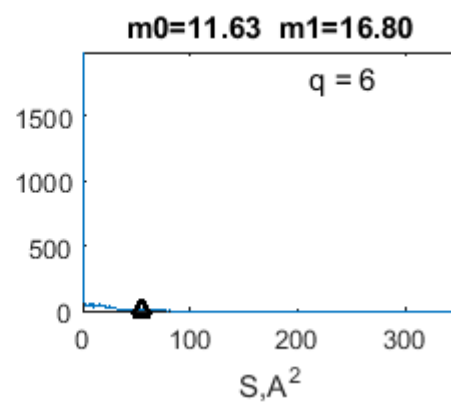
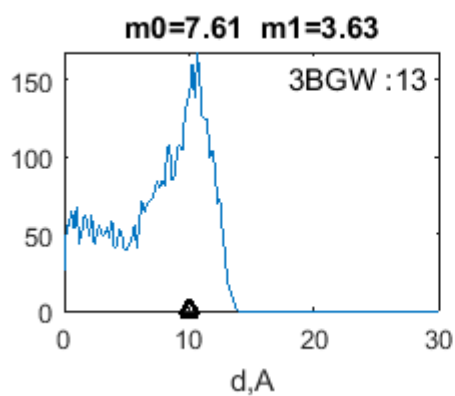
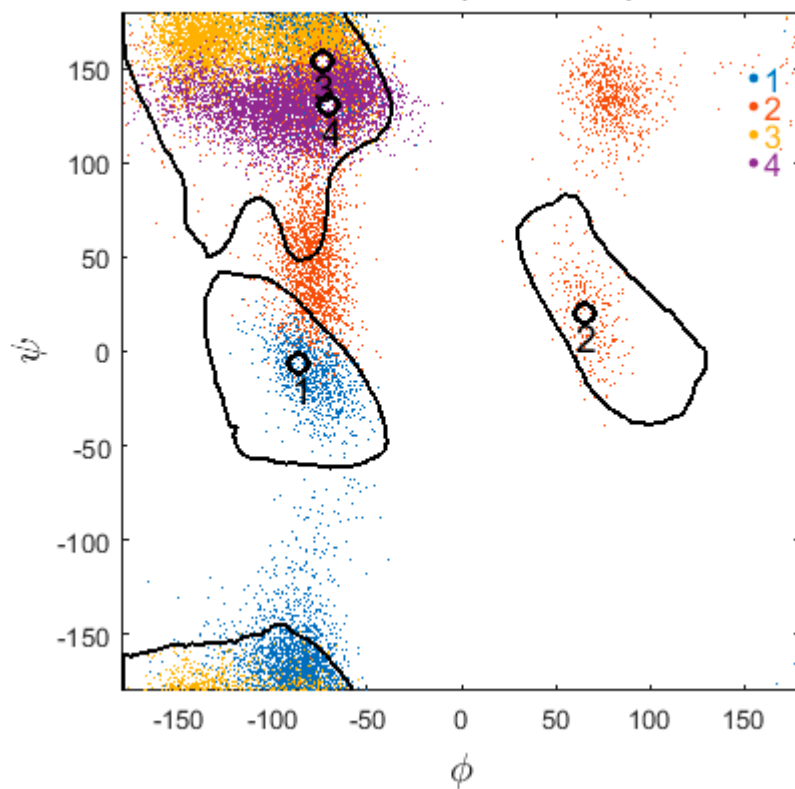
51 1Q3Q : 4 $\xi_p=100.0\%$ $S_p=100.0\%$



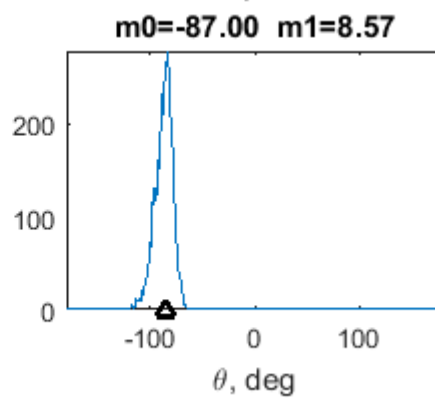
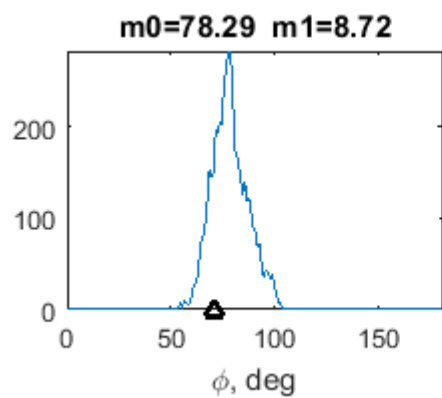
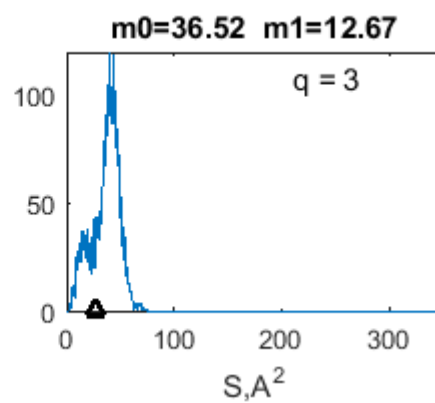
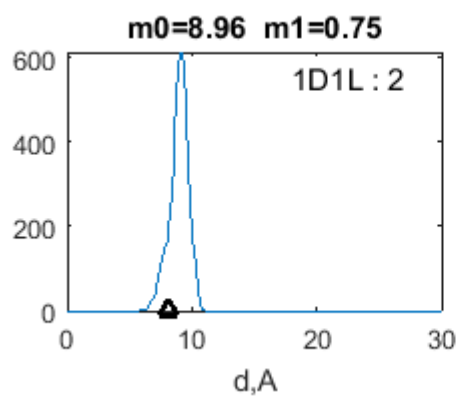
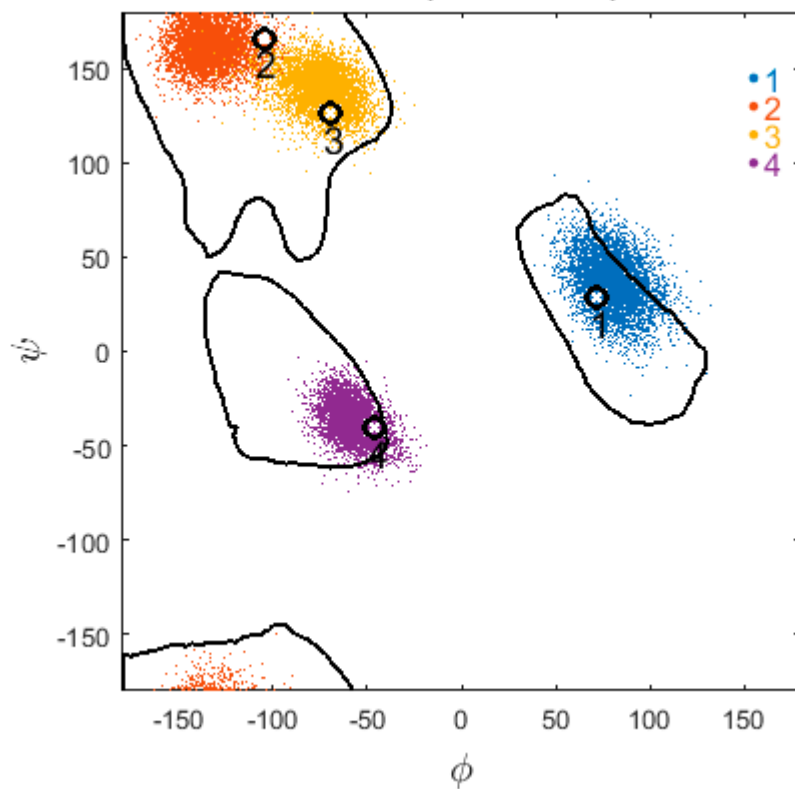
49 2PSN : 5 $\xi_p=100.0\%$ $S_p=100.0\%$



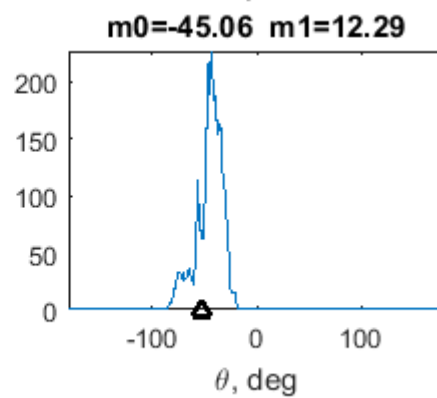
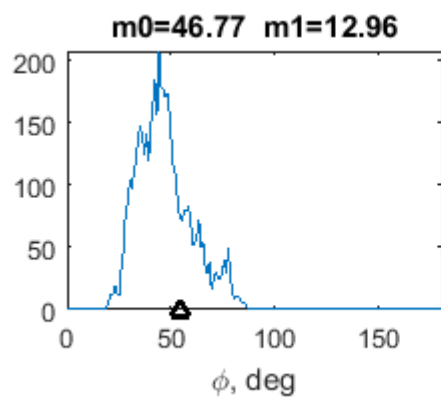
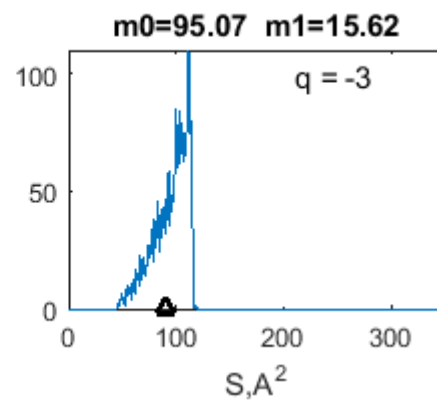
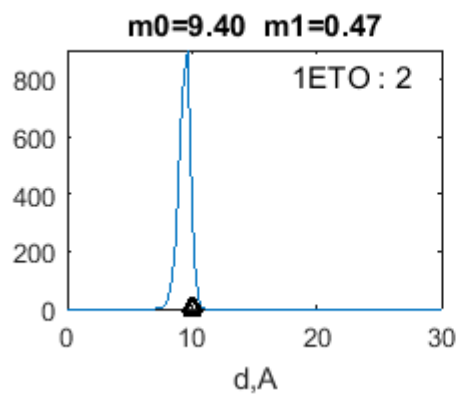
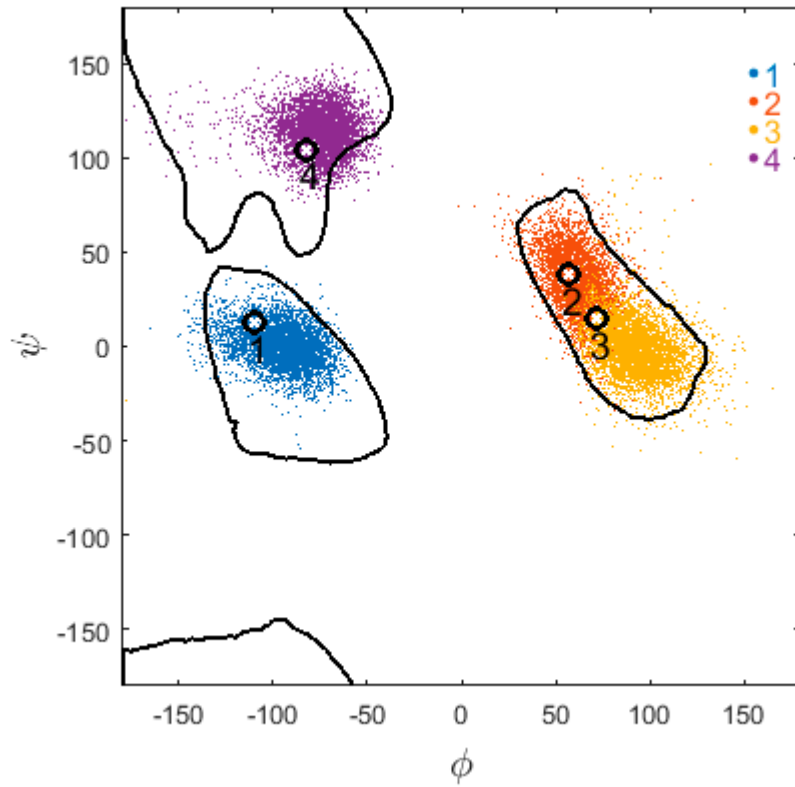
45 3BGW : 13 $\xi_p=36.3\%$ $S_p=66.3\%$



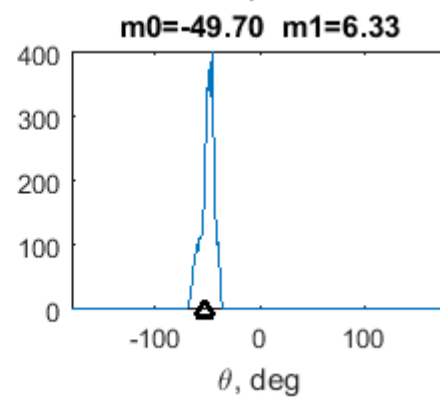
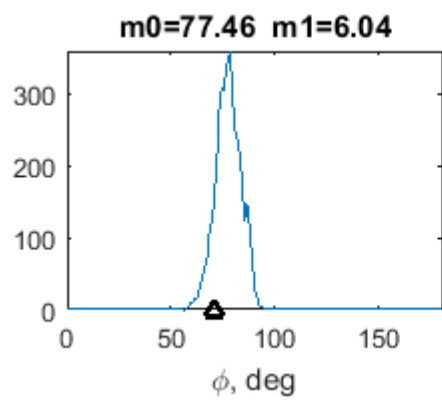
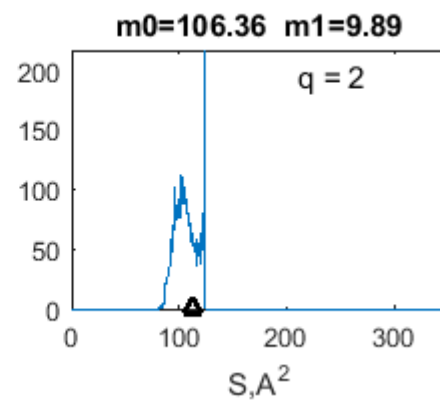
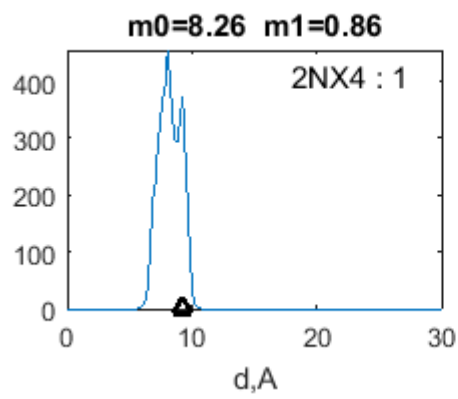
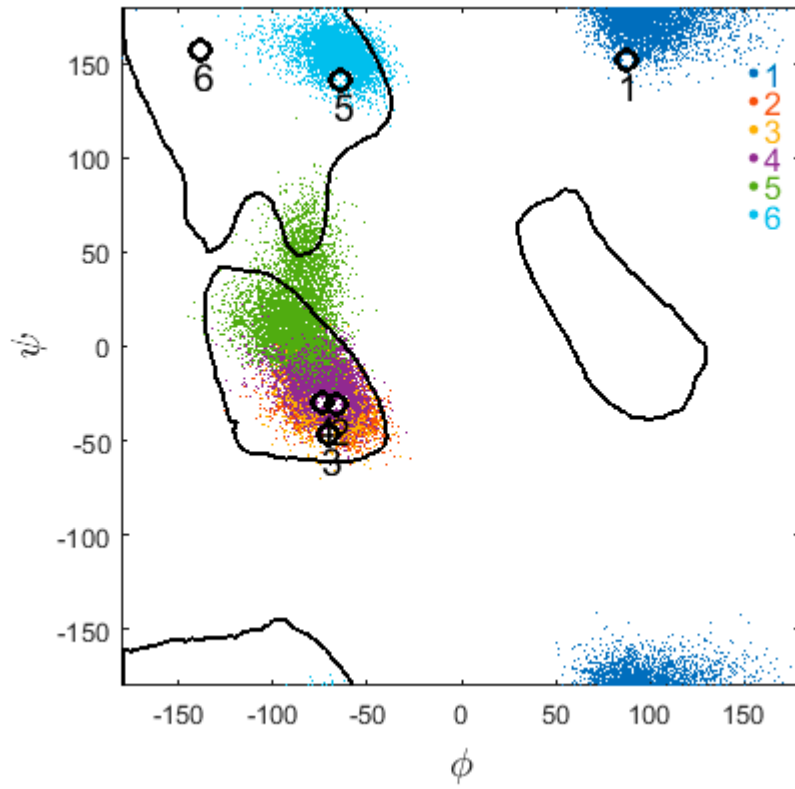
52 1D1L : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



43 1ETO : 2 $\xi_p=100.0\%$ $S_p=100.0\%$



54 2NX4 : 1 $\xi_p=100.0\%$ $S_p=100.0\%$



53 2OEM : 19 $\xi_p=97.9\%$ $S_p=100.0\%$

